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- **KWAK, Yoonhyun**
16678 Gyeonggi-do (KR)
- **KIM, Juhyun**
16678 Gyeonggi-do (KR)
- **PARK, Sangho**
16678 Gyeonggi-do (KR)
- **LEE, Sunghun**
16678 Gyeonggi-do (KR)
- **YI, Jeoungin**
16678 Gyeonggi-do (KR)

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(71) Applicant: **Samsung Electronics Co., Ltd.**
Suwon-si 16677 (KR)

(74) Representative: **Elkington and Fife LLP**
Prospect House
8 Pembroke Road
Sevenoaks, Kent TN13 1XR (GB)

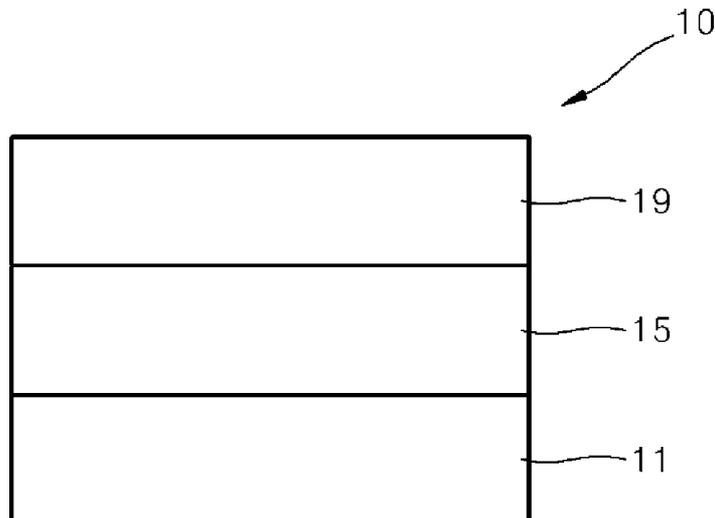
(72) Inventors:
• **LEE, Sunyoung**
16678 Gyeonggi-do (KR)

(54) **ORGANOMETALLIC COMPOUND, ORGANIC LIGHT-EMITTING DEVICE INCLUDING ORGANOMETALLIC COMPOUND, AND DIAGNOSTIC COMPOSITION INCLUDING ORGANOMETALLIC COMPOUND**

(57) Provided are an organometallic compound represented by Formula 1, an organic light-emitting device including the organometallic compound, and a diagnostic composition including the organometallic compound:



wherein, in Formula 1, M, L₁, L₂, n₁ and n₂ may each be understood by referring to the descriptions thereof provided herein.



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Description

FIELD OF THE INVENTION

5 [0001] The present disclosure relates to an organometallic compound, an organic light-emitting device including the organometallic compound, and a diagnostic composition including the organometallic compound.

BACKGROUND OF THE INVENTION

10 [0002] Organic light-emitting devices (OLEDs) are self-emission devices which produce full-color images. In addition, OLEDs have wide viewing angles and exhibit excellent driving voltage and response speed characteristics.

[0003] OLEDs include an anode, a cathode, and an organic layer between the anode and the cathode and including an emission layer. A hole transport region may be between the anode and the emission layer, and an electron transport region may be between the emission layer and the cathode. Holes provided from the anode may move toward the emission layer through the hole transport region, and electrons provided from the cathode may move toward the emission layer through the electron transport region. The holes and the electrons recombine in the emission layer to produce excitons. These excitons transit from an excited state to a ground state to thereby generate light.

15 [0004] Further, light-emitting compounds, e.g., phosphorescence-emitting compounds, can also be used to monitor, sense, or detect biological materials, including a variety of cells and proteins.

20 SUMMARY OF THE INVENTION

[0005] Provided are an organometallic compound, an organic light-emitting device including the organometallic compound, and a diagnostic composition including the organometallic compound.

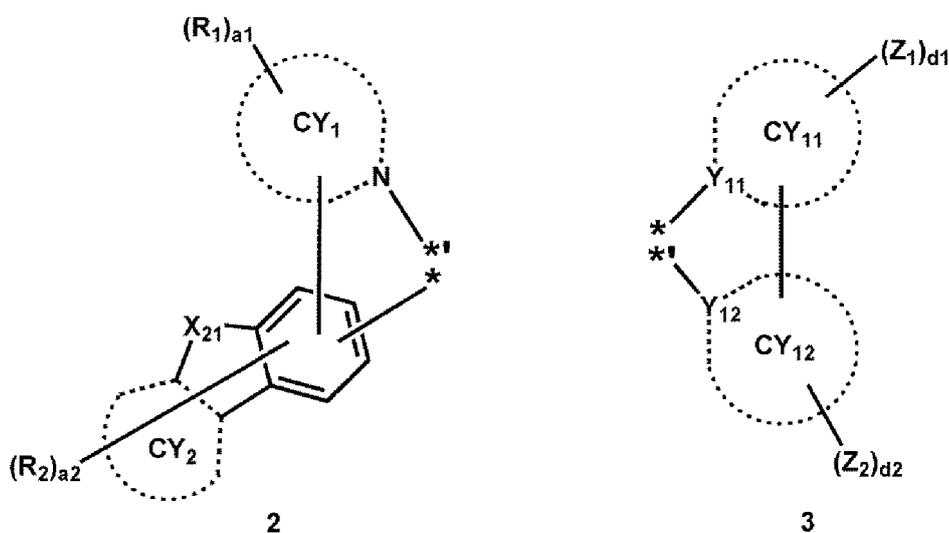
25 [0006] Additional aspects will be set forth in part in the description which follows and, in part, will be apparent from the description, or may be learned by practice of the presented embodiments of the disclosure.

[0007] According an aspect of an embodiment, an organometallic compound is represented by Formula 1.



wherein, in Formula 1,

- M is a transition metal,
- L₁ is a ligand represented by Formula 2,
- 35 L₂ is a ligand represented by Formula 3,
- n₁ and n₂ are each 1 or 2, and the sum of n₁ and n₂ is 3,
- L₁ is different from L₂,



wherein, in Formulae 2 and 3,

Y₁₁ is N, and Y₁₂ is C,

ring CY₁ and ring CY₁₁ are each independently a C₁-C₃₀ heterocyclic group,

ring CY₂ and ring CY₁₂ are each independently a C₅-C₃₀ carbocyclic group or a C₁-C₃₀ heterocyclic group,

X₂₁ is O, S, Se, N(R₂₈), C(R₂₈)(R₂₉), or Si(R₂₈)(R₂₉),

5 R₁, R₂, R₂₈, R₂₉, Z₁, and Z₂ are each independently deuterium, -F, -Cl, -Br, -I, -SF₅, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C₁-C₆₀ alkyl group, a substituted or unsubstituted C₂-C₆₀ alkenyl group, a substituted or unsubstituted C₂-C₆₀ alkynyl group, a substituted or unsubstituted C₁-C₆₀ alkoxy group, a substituted or unsubstituted C₆-C₃₀ unsaturated carbocyclic group, a substituted or unsubstituted C₂-C₃₀ unsaturated heterocyclic group, -N(Q₁)(Q₂), -Si(Q₃)(Q₄)(Q₅), -Ge(Q₃)(Q₄)(Q₅), -B(Q₆)(Q₇), -P(=O)(Q₈)(Q₉), or -P(Q₈)(Q₉),

10 a₁, a₂, and d₁ are each independently an integer from 0 to 10, wherein, when a₁ is 2 or greater, at least two R₁(s) may be identical to or different from each other, when a₂ is 2 or greater, at least two R₂(s) may be identical to or different from each other, and when d₁ is 2 or greater, at least two Z₁(s) may be identical to or different from each other, the sum of a₁ and a₂ is 1 or greater,

15 d₂ is an integer from 1 to 10, wherein, when d₂ is 2 or greater, at least two Z₂(s) are identical to or different from each other,

at least two selected from a plurality of R₁(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

20 at least two selected from a plurality of R₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from a plurality of Z₁(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

25 at least two selected from a plurality of Z₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from R₁(s), R₂(s), Z₁(s), and Z₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}.

R_{10a} is understood by referring to the description of R₁ provided herein,

30 * and *' may each indicate a binding site to M in Formula 1, and

a substituent of the substituted C₁-C₆₀ alkyl group, the substituted C₂-C₆₀ alkenyl group, the substituted C₂-C₆₀ alkynyl group, the substituted C₁-C₆₀ alkoxy group, the substituted C₆-C₃₀ unsaturated carbocyclic group, and the substituted C₂-C₃₀ unsaturated heterocyclic group is:

35 deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or a C₁-C₆₀ alkoxy group,

40 a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or a C₁-C₆₀ alkoxy group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₆-C₃₀ unsaturated carbocyclic group, a C₂-C₃₀ unsaturated heterocyclic group, -N(Q₁₁)(Q₁₂), -Si(Q₁₃)(Q₁₄)(Q₁₅), -Ge(Q₁₃)(Q₁₄)(Q₁₅), -B(Q₁₆)(Q₁₇), -P(=O)(Q₁₈)(Q₁₉), -P(Q₁₈)(Q₁₉), or any combination thereof,

45 a C₆-C₃₀ unsaturated carbocyclic group or a C₂-C₃₀ unsaturated heterocyclic group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, a C₁-C₆₀ alkoxy group, a C₆-C₃₀ unsaturated carbocyclic group, a C₂-C₃₀ unsaturated heterocyclic group, -N(Q₂₁)(Q₂₂), -Si(Q₂₃)(Q₂₄)(Q₂₅), -Ge(Q₂₃)(Q₂₄)(Q₂₅), -B(Q₂₆)(Q₂₇), -P(=O)(Q₂₈)(Q₂₉), -P(Q₂₈)(Q₂₉), or any combination thereof,

50 -N(Q₃₁)(Q₃₂), -Si(Q₃₃)(Q₃₄)(Q₃₅), -Ge(Q₃₃)(Q₃₄)(Q₃₅), -B(Q₃₆)(Q₃₇), -P(=O)(Q₃₈)(Q₃₉), or -P(Q₃₈)(Q₃₉), or any combination thereof,

55 wherein Q₁ to Q₉, Q₁₁ to Q₁₉, Q₂₁ to Q₂₉, and Q₃₁ to Q₃₉ are each independently hydrogen, deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, a C₁-C₆₀ alkoxy group,

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or a C₆-C₃₀ unsaturated carbocyclic group or C₂-C₃₀ unsaturated heterocyclic group, each unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof.

5 [0008] According to an aspect of another embodiment, an organic light-emitting device includes a first electrode, a second electrode, and an organic layer disposed between the first electrode and the second electrode and including an emission layer, the organic layer including at least one organometallic compound represented by Formula 1.

[0009] In the organic layer, the organometallic compound included in the emission layer may serve as a dopant.

10 [0010] According to an aspect of still another embodiment, a diagnostic composition may include at least one organometallic compound represented by Formula 1.

BRIEF DESCRIPTION OF THE DRAWING

[0011] The above and other aspects, features, and advantages of certain embodiments of the disclosure will be more apparent from the following description taken in conjunction with the accompanying drawings, in which

15 The FIGURE is a schematic cross-sectional view of an organic light-emitting device according to an embodiment.

DETAILED DESCRIPTION OF THE EMBODIMENTS

20 [0012] Reference will now be made in detail to embodiments, examples of which are illustrated in the accompanying drawings, wherein like reference numerals refer to like elements throughout. In this regard, the present embodiments may have different forms and should not be construed as being limited to the descriptions set forth herein. Accordingly, the embodiments are merely described below, by referring to the figures, to explain aspects. As used herein, the term "and/or" includes any and all combinations of one or more of the associated listed items. Expressions such as "at least one of," when preceding a list of elements, modify the entire list of elements and do not modify the individual elements

25 of the list.
[0013] It will be understood that when an element is referred to as being "on" another element, it can be directly on the other element or intervening elements may be present therebetween. In contrast, when an element is referred to as being "directly on" another element, there are no intervening elements present.

30 [0014] It will be understood that, although the terms "first," "second," "third" etc. may be used herein to describe various elements, components, regions, layers and/or sections, these elements, components, regions, layers and/or sections should not be limited by these terms. These terms are only used to distinguish one element, component, region, layer or section from another element, component, region, layer or section. Thus, "a first element," "component," "region," "layer" or "section" discussed below could be termed a second element, component, region, layer or section without departing from the teachings herein.

35 [0015] The terminology used herein is for the purpose of describing particular embodiments only and is not intended to be limiting. As used herein, "a," "an," "the," and "at least one" do not denote a limitation of quantity, and are intended to cover both the singular and plural, unless the context clearly indicates otherwise. For example, "an element" has the same meaning as "at least one element," unless the context clearly indicates otherwise.

40 [0016] "Or" means "and/or." As used herein, the term "and/or" includes any and all combinations of one or more of the associated listed items. It will be further understood that the terms "comprises" and/or "comprising," or "includes" and/or "including" when used in this specification, specify the presence of stated features, regions, integers, steps, operations, elements, and/or components, but do not preclude the presence or addition of one or more other features, regions, integers, steps, operations, elements, components, and/or groups thereof.

45 [0017] Furthermore, relative terms, such as "lower" or "bottom" and "upper" or "top," may be used herein to describe one element's relationship to another element as illustrated in the Figures. It will be understood that relative terms are intended to encompass different orientations of the device in addition to the orientation depicted in the Figures. For example, if the device in one of the figures is turned over, elements described as being on the "lower" side of other elements would then be oriented on "upper" sides of the other elements. The exemplary term "lower," can therefore, encompass both an orientation of "lower" and "upper," depending on the particular orientation of the figure. Similarly,

50 if the device in one of the figures is turned over, elements described as "below" or "beneath" other elements would then be oriented "above" the other elements. The exemplary terms "below" or "beneath" can, therefore, encompass both an orientation of above and below.
[0018] "About" or "approximately" as used herein is inclusive of the stated value and means within an acceptable range of deviation for the particular value as determined by one of ordinary skill in the art, considering the measurement in question and the error associated with measurement of the particular quantity (i.e., the limitations of the measurement system). For example, "about" can mean within one or more standard deviations, or within $\pm 30\%$, 20% , 10% or 5% of the stated value.

55 [0019] Unless otherwise defined, all terms (including technical and scientific terms) used herein have the same meaning

as commonly understood by one of ordinary skill in the art to which this disclosure belongs It will be further understood that terms, such as those defined in commonly used dictionaries, should be interpreted as having a meaning that is consistent with their meaning in the context of the relevant art and the present disclosure, and will not be interpreted in an idealized or overly formal sense unless expressly so defined herein.

[0020] Exemplary embodiments are described herein with reference to cross section illustrations that are schematic illustrations of idealized embodiments As such, variations from the shapes of the illustrations as a result, for example, of manufacturing techniques and/or tolerances, are to be expected Thus, embodiments described herein should not be construed as limited to the particular shapes of regions as illustrated herein but are to include deviations in shapes that result, for example, from manufacturing. For example, a region illustrated or described as flat may, typically, have rough and/or nonlinear features Moreover, sharp angles that are illustrated may be rounded Thus, the regions illustrated in the figures are schematic in nature and their shapes are not intended to illustrate the precise shape of a region and are not intended to limit the scope of the present claims.

[0021] According to an aspect, an organometallic compound may be represented by Formula 1:



[0022] In Formula 1, M may be a transition metal.

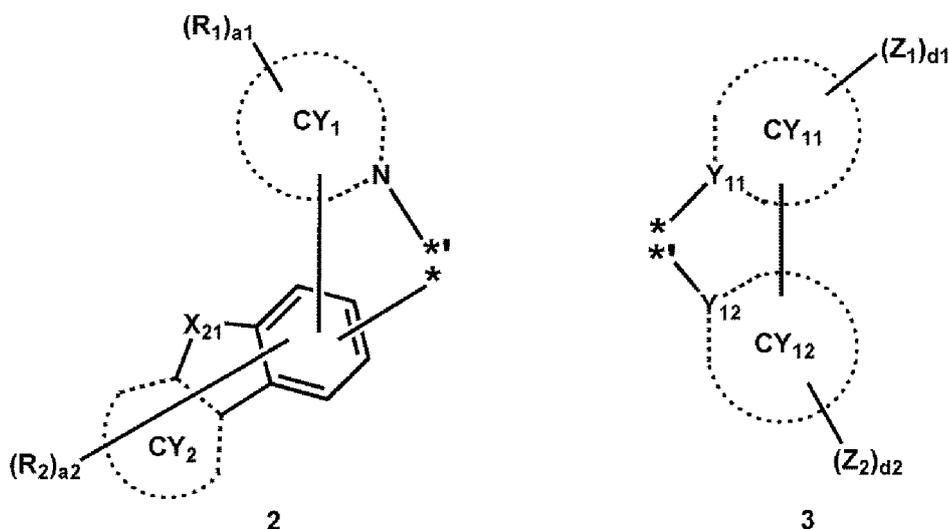
[0023] In some embodiments, M may be a first-row transition metal, a second-row transition metal, or a third-row transition metal.

[0024] In some embodiments, M may be iridium (Ir), platinum (Pt), osmium (Os), titanium (Ti), zirconium (Zr), hafnium (Hf), europium (Eu), terbium (Tb), thulium (Tm), or rhodium (Rh).

[0025] In some embodiments, M may be Ir, Pt, Os, or Rh.

[0026] In one or more embodiments, M may be iridium (Ir).

[0027] L₁ in Formula 1 may be a ligand represented by Formula 2, and L₂ may be a ligand represented by Formula 3:



[0028] Formulae 2 and 3 may each be understood by referring to the descriptions thereof provided herein.

[0029] n₁ and n₂ in Formula 1 may respectively indicate the number of L₁(s) and L₂(s), and n₁ and n₂ may each independently be 1 or 2. When n₁ is 2, two L₁(s) may be identical to or different from each other, and when n₂ is 2, two L₂(s) may be identical to or different from each other. The sum of n₁ and n₂ may be 3.

[0030] L₁ and L₂ in Formula 1 may be different from each other. That is, the organometallic compound represented by Formula 1 may be a heteroleptic complex.

[0031] In Formula 3, Y₁₁ may be N, and Y₁₂ may be C.

[0032] In Formulae 2 and 3, ring CY₁ and ring CY₁₁ may each independently be a C₁-C₃₀ heterocyclic group, and ring CY₂ and ring CY₁₂ may each independently be a C₅-C₃₀ carbocyclic group or a C₁-C₃₀ heterocyclic group. Ring CY₁ and ring CY₁₁ may respectively be the lowest unoccupied molecular orbital (LUMO) parts in the ligands represented by Formulae 2 and 3, and a condensed ring, with which ring CY₂ is condensed, and ring CY₁₂ may respectively be the highest occupied molecular orbital (HOMO) parts in the ligands represented by Formulae 2 and 3.

[0033] In some embodiments, ring CY₁ and ring CY₁₁ may each independently be an azaindole group, an azabenzoborole group, an azabenzophosphole group, an azaindene group, an azabenzosilole group, an azabenzogermole group, an azabenzothiophene group, an azabenzoselenophene group, an azabenzofuran group, an azacarbazole group,

an azadibenzoborole group, an azadibenzophosphole group, an azafluorene group, an azadibenzosilole group, an azadibenzogermole group, an azadibenzothiophene group, an azadibenzoselenophene group, an azadibenzofuran group, an azadibenzothiophene 5-oxide group, an aza-9H-fluorene-9-one group, an azadibenzothiophene 5,5-dioxide group, a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a pyrrole group, a pyrazole group, an imidazole group, a triazole group, an oxazole group, an isooxazole group, a thiazole group, an isothiazole group, an oxadiazole group, a thiadiazole group, a benzopyrazole group, a benzimidazole group, a benzoxazole group, a benzothiazole group, a benzoxadiazole group, a benzothiadiazole group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group.

[0034] In some embodiments, ring CY_2 and ring CY_{12} may each independently be a cyclopentene group, a cyclohexene group, a benzene group, a naphthalene group, an anthracene group, a phenanthrene group, a triphenylene group, a pyrene group, a chrysene group, a cyclopentadiene group, a 1,2,3,4-tetrahydronaphthalene group, a thiophene group, a furan group, an indole group, a borole group, a silole group, a germole group, a phosphole group, a selenophene group, a benzoborole group, a benzophosphole group, an indene group, a benzosilole group, a benzogermole group, a benzothiophene group, a benzoselenophene group, a benzofuran group, a carbazole group, a dibenzoborole group, a dibenzophosphole group, a fluorene group, a dibenzosilole group, a dibenzogermole group, a dibenzothiophene group, a dibenzoselenophene group, a dibenzofuran group, a dibenzothiophene 5-oxide group, a 9H-fluorene-9-one group, a dibenzothiophene 5,5-dioxide group, an azaindole group, an azabenzoborole group, an azabenzophosphole group, an azabenzoselenophene group, an azabenzosilole group, an azabenzogermole group, an azadibenzothiophene group, an azabenzoselenophene group, an azabenzofuran group, an azacarbazole group, an azadibenzoborole group, an azadibenzophosphole group, an azafluorene group, an azadibenzosilole group, an azadibenzogermole group, an azadibenzothiophene group, an azadibenzoselenophene group, an azadibenzofuran group, an azadibenzothiophene 5-oxide group, an aza-9H-fluorene-9-one group, an azadibenzothiophene 5,5-dioxide group, a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a pyrrole group, a pyrazole group, an imidazole group, a triazole group, an oxazole group, an isooxazole group, a thiazole group, an isothiazole group, an oxadiazole group, a thiadiazole group, a benzopyrazole group, a benzimidazole group, a benzoxazole group, a benzothiazole group, a benzoxadiazole group, a benzothiadiazole group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group.

[0035] In some embodiments, ring CY_1 and ring CY_{11} may each independently be a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group, and ring CY_2 and ring CY_{12} may each independently be a benzene group, a naphthalene group, an anthracene group, a phenanthrene group, a triphenylene group, a pyrene group, a chrysene group, a 1,2,3,4-tetrahydronaphthalene group, a thiophene group, a furan group, an indole group, a borole group, a silole group, a germole group, a phosphole group, a selenophene group, a benzoborole group, a benzophosphole group, an indene group, a benzosilole group, a benzogermole group, a benzothiophene group, a benzoselenophene group, a benzofuran group, a carbazole group, a dibenzoborole group, a dibenzophosphole group, a fluorene group, a dibenzosilole group, a dibenzogermole group, a dibenzothiophene group, a dibenzoselenophene group, a dibenzofuran group, a dibenzothiophene 5-oxide group, a 9H-fluorene-9-one group, a dibenzothiophene 5,5-dioxide group, a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group.

[0036] In one or more embodiments, ring CY_1 and ring CY_{11} may each independently be a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group, and ring CY_2 and ring CY_{12} may each independently be a benzene group, a naphthalene group, or a 1,2,3,4-tetrahydronaphthalene group.

[0037] In one or more embodiments, ring CY_1 and ring CY_{11} may each be a pyridine group, and ring CY_2 and ring CY_{12} may be a benzene group.

[0038] In Formula 2, X_{21} may be O, S, Se, $N(R_{28})$, $C(R_{28})(R_{29})$, or $Si(R_{28})(R_{29})$.

[0039] In some embodiments, X_{21} may be O or S.

[0040] In Formulae 2 and 3, R_1 , R_2 , R_{28} , R_{29} , Z_1 , and Z_2 may each independently be deuterium, -F, -Cl, -Br, -I, -SF₅, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C₁-C₆₀ alkyl group, a substituted or unsubstituted C₂-C₆₀ alkenyl group, a substituted or unsubstituted C₂-C₆₀ alkynyl group, a substituted or unsubstituted C₁-C₆₀ alkoxy group, a substituted or unsubstituted C₆-C₃₀ unsaturated carbocyclic group, a substituted or unsubstituted C₂-C₃₀ unsaturated heterocyclic group, -N(Q₁)(Q₂), -Si(Q₃)(Q₄)(Q₅), -Ge(Q₃)(Q₄)(Q₅), -B(Q₆)(Q₇), -P(=O)(Q₈)(Q₉), or -P(Q₈)(Q₉), wherein Q₁ to Q₉ may

respectively be understood by referring to the descriptions of Q₁ to Q₉ provided herein.

[0041] In some embodiments, R₁, R₂, R₂₈, R₂₉, Z₁, and Z₂ may each independently be:

5 deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, -SF₅, a C₁-C₂₀ alkyl group, a C₁-C₂₀ alkenyl group, or a C₁-C₂₀ alkoxy group; a C₁-C₂₀ alkyl group, a C₁-C₂₀ alkenyl group, or a C₁-C₂₀ alkoxy group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₁₀ alkyl group, a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, or any combination thereof;

10 a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, a benzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, an imidazopyrimidinyl group, an azacarbazolyl group, an azadibenzofuranyl group, or an azadibenzothiophenyl group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₂₀ alkyl group, a deuterated C₂-C₂₀ alkyl group, a C₁-C₂₀ alkoxy group, a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, an imidazopyrimidinyl group, an azacarbazolyl group, an azadibenzofuranyl group, an azadibenzothiophenyl group, or any combination thereof; or

15 -N(Q₁)(Q₂), -Si(Q₃)(Q₄)(Q₅), -Ge(Q₃)(Q₄)(Q₅), -B(Q₆)(Q₇), -P(=O)(Q₈)(Q₉), or -P(Q₈)(Q₉),

20 wherein Q₁ to Q₉ may each independently be:

25 deuterium, -F, -CH₃, -CD₃, -CD₂H, -CDH₂, -CH₂CH₃, -CH₂CD₃, -CH₂CD₂H, -CH₂CDH₂, -CHDCH₃, -CHDCD₂H, -CHDCDH₂, -CHDCD₃, -CD₂CD₃, -CD₂CD₂H, -CD₂CDH₂, -CF₃, -CF₂H, -CFH₂, -CH₂CF₃, -CH₂CF₂H, -CH₂CFH₂, -CHFCH₃, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CF₂CF₃, -CF₂CF₂H, or -CF₂CFH₂; or

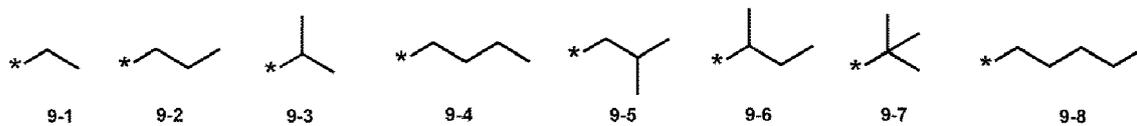
30 an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an isobutyl group, a tert-butyl group, an n-pentyl group, a tert-pentyl group, a neopentyl group, an isopentyl group, a sec-pentyl group, a 3-pentyl group, a sec-isopentyl group, a phenyl group, a biphenyl group, or a naphthyl group, each unsubstituted or substituted with deuterium, -F, a C₁-C₁₀ alkyl group, a phenyl group, or any combination thereof.

35 **[0042]** In one or more embodiments, in Formulae 2 and 3, R₁, R₂, R₂₈, R₂₉, Z₁, and Z₂ may each independently be deuterium, -F, -CH₃, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a C₁-C₁₀ alkenyl group, a C₁-C₁₀ alkoxy group, a group represented by one of Formulae 9-1 to 9-39, a group represented by one of Formulae 9-1 to 9-39 in which at least one hydrogen is substituted with deuterium, a group represented by one of Formulae 9-1 to 9-39 in which at least one hydrogen is substituted with -F, a group represented by one of Formulae 10-1 to 10-112, a group represented by one of Formulae 10-1 to 10-112 in which at least one hydrogen is substituted with deuterium, a group represented by one of Formulae 10-1 to 10-112 in which at least one hydrogen is substituted with -F, a group represented by one of Formulae 10-201 to 10-350, a group represented by one of Formulae 10-201 to 10-350 in which at least one hydrogen is substituted with deuterium, a group represented by one of Formulae 10-201 to 10-350 in which at least one hydrogen is substituted

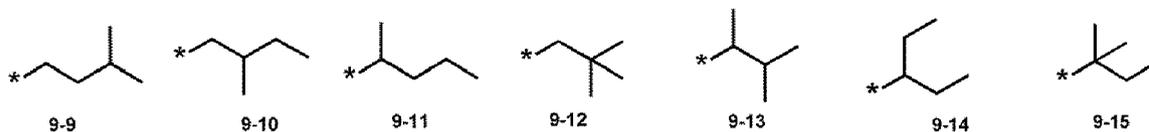
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with -F, -Si(Q₃)(Q₄)(Q₅), or -Ge(Q₃)(Q₄)(Q₅), wherein Q₃ to Q₅ may respectively be understood by referring to the descriptions of Q₃ to Q₅ provided herein:

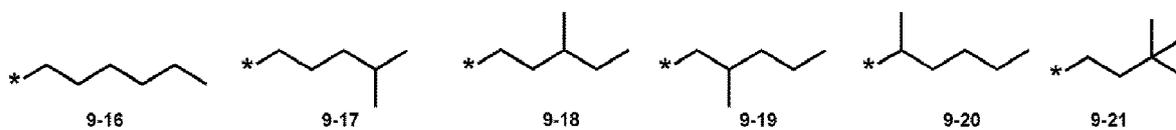
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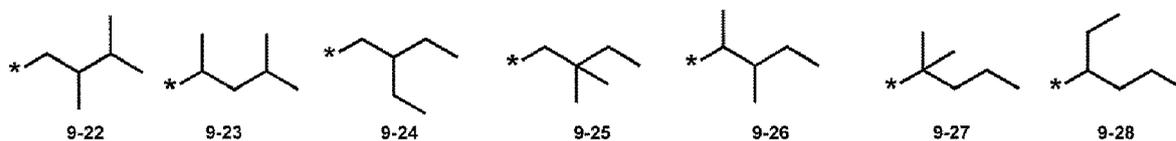
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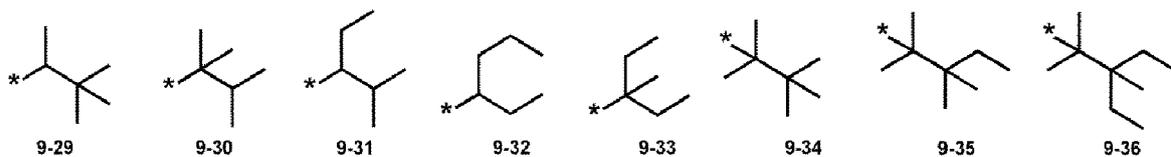
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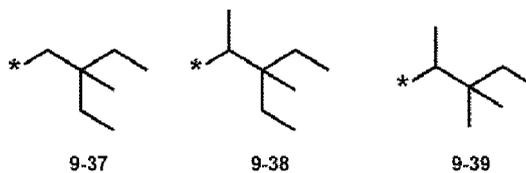


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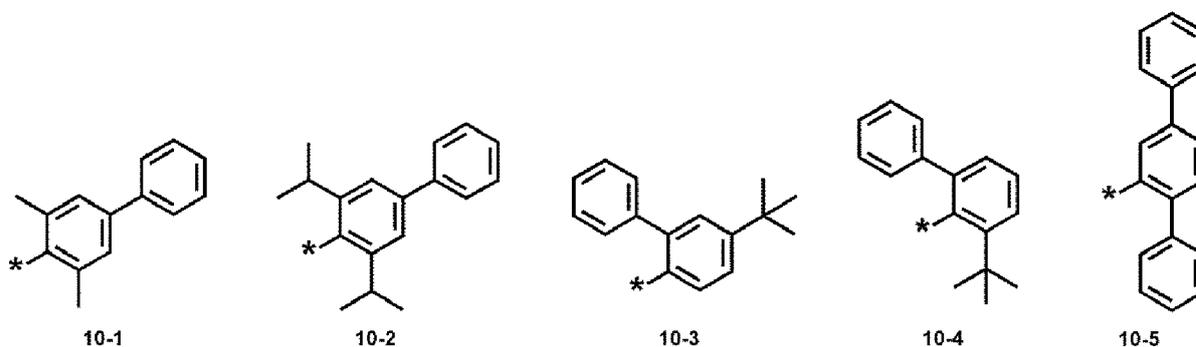
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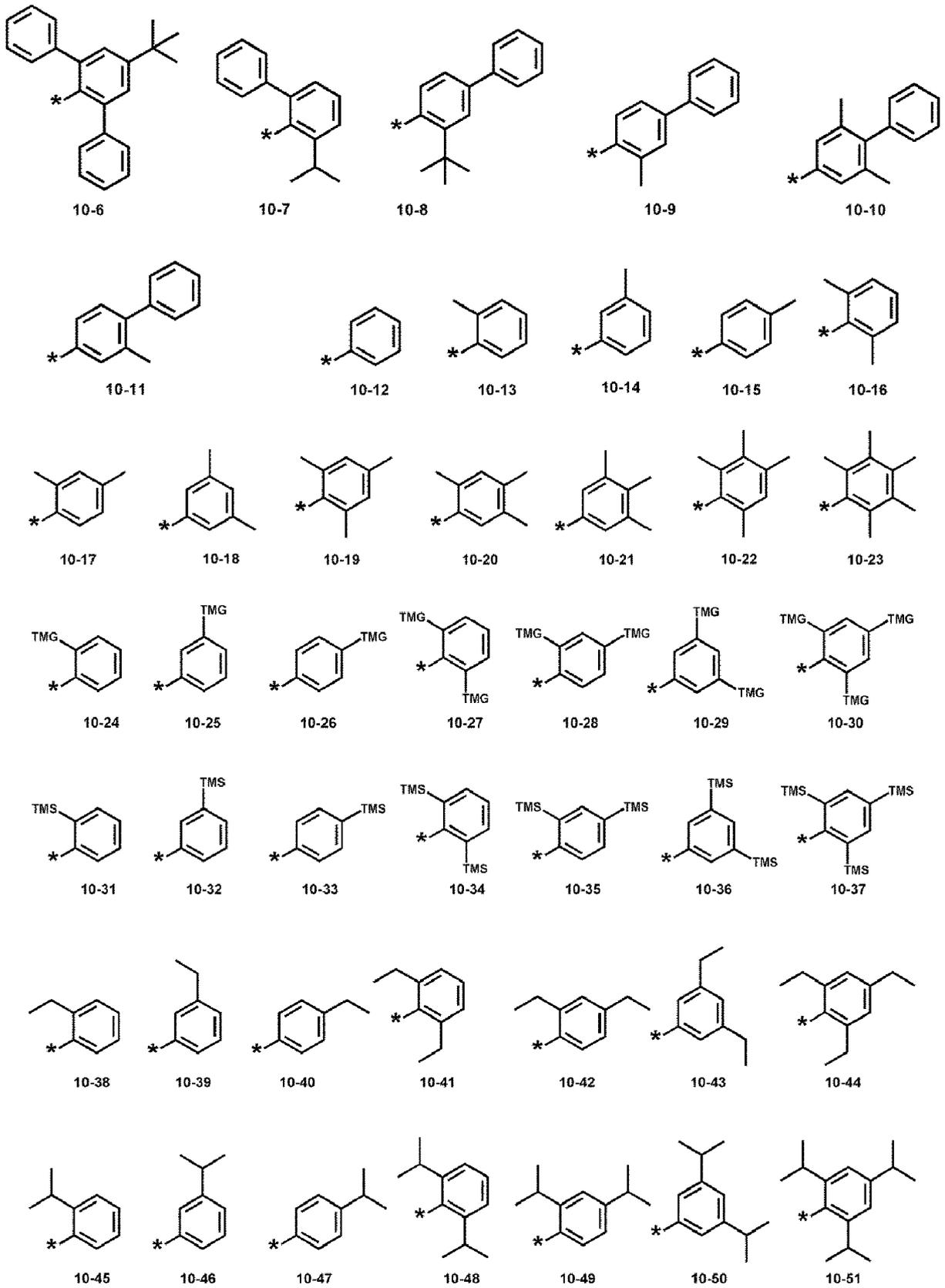
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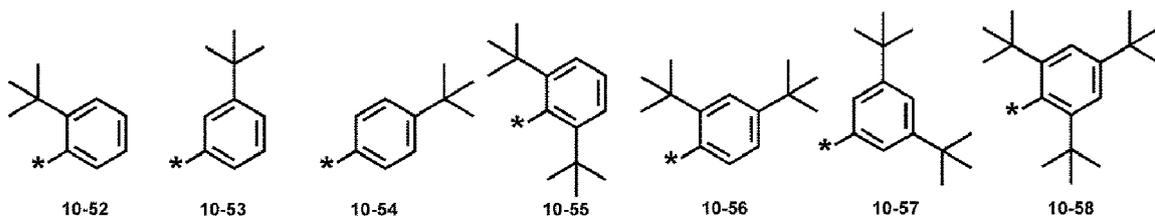
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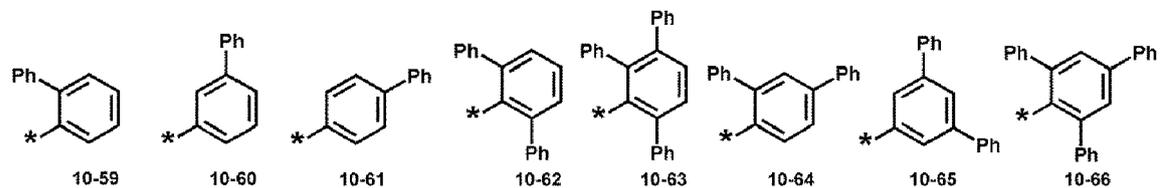
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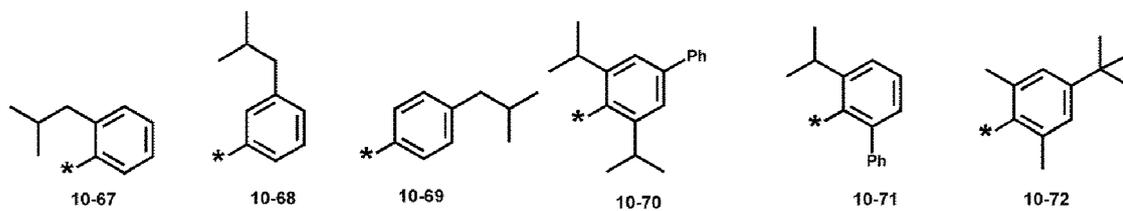


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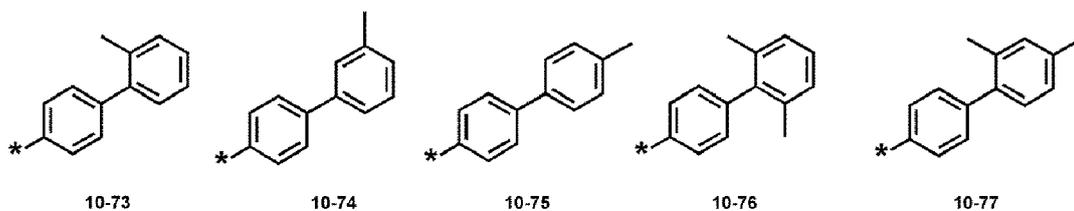
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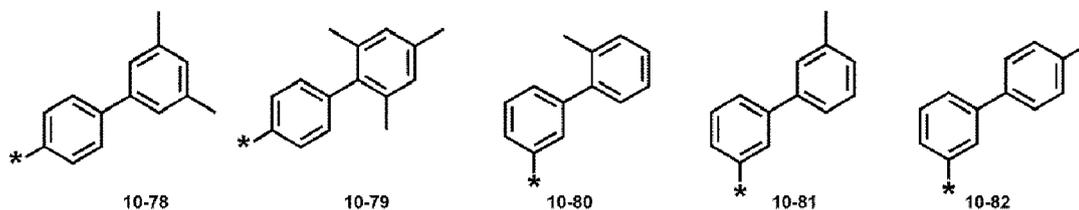


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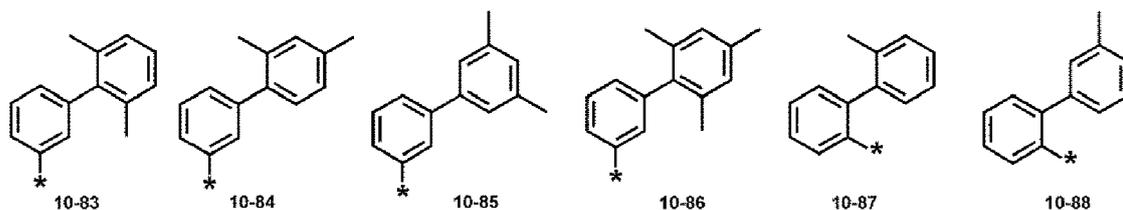


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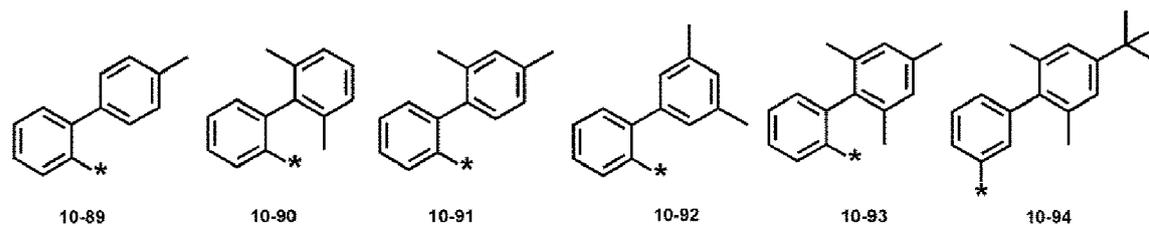


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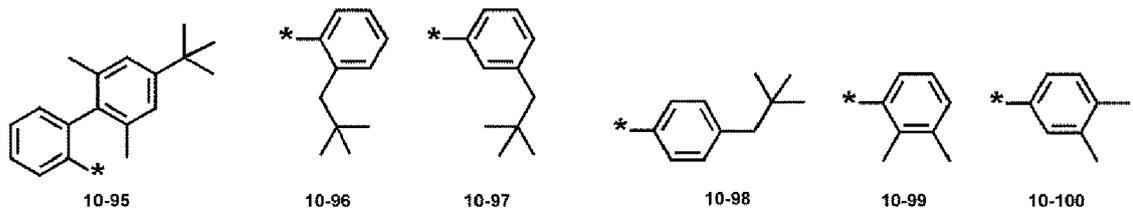


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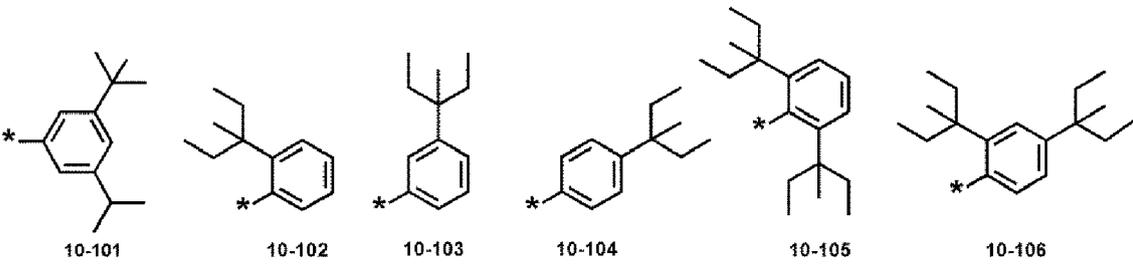


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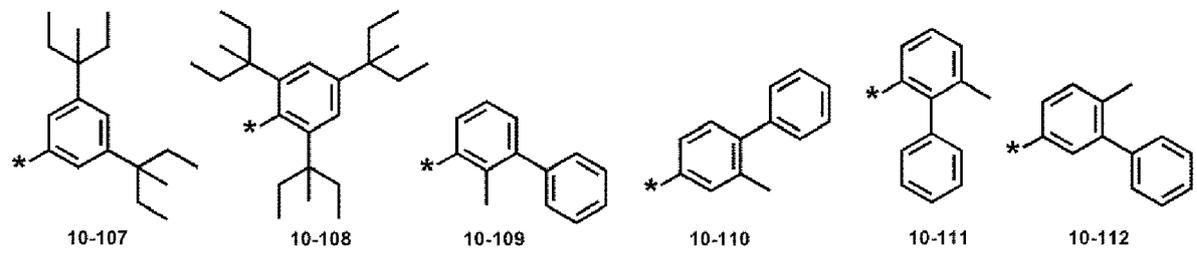


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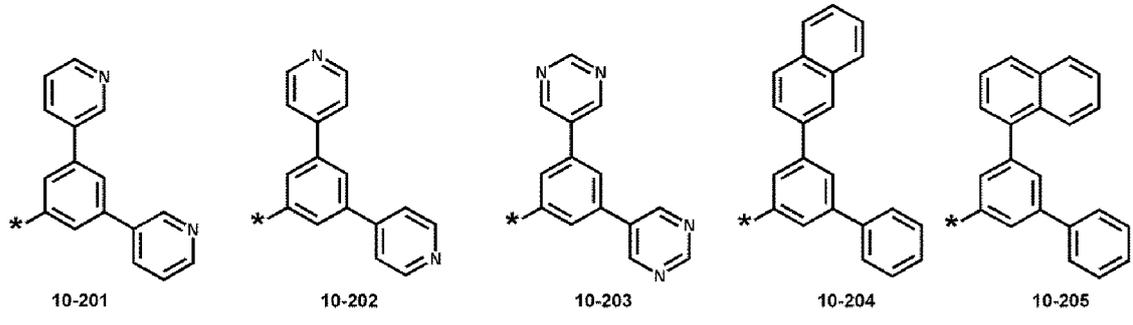
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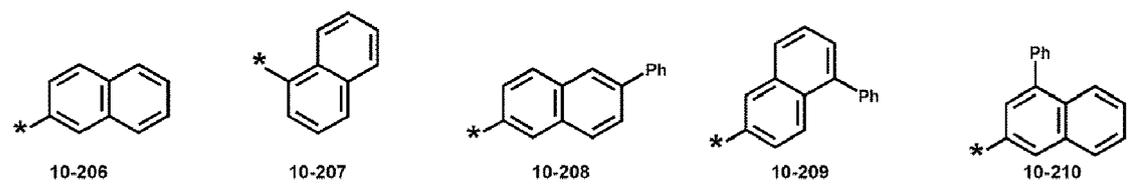
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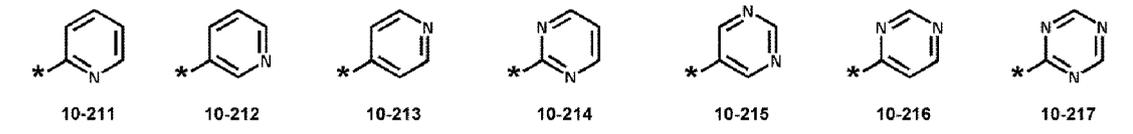
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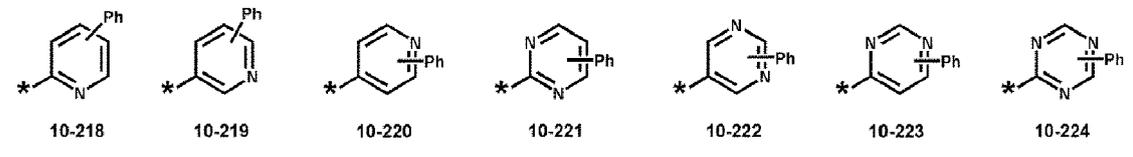


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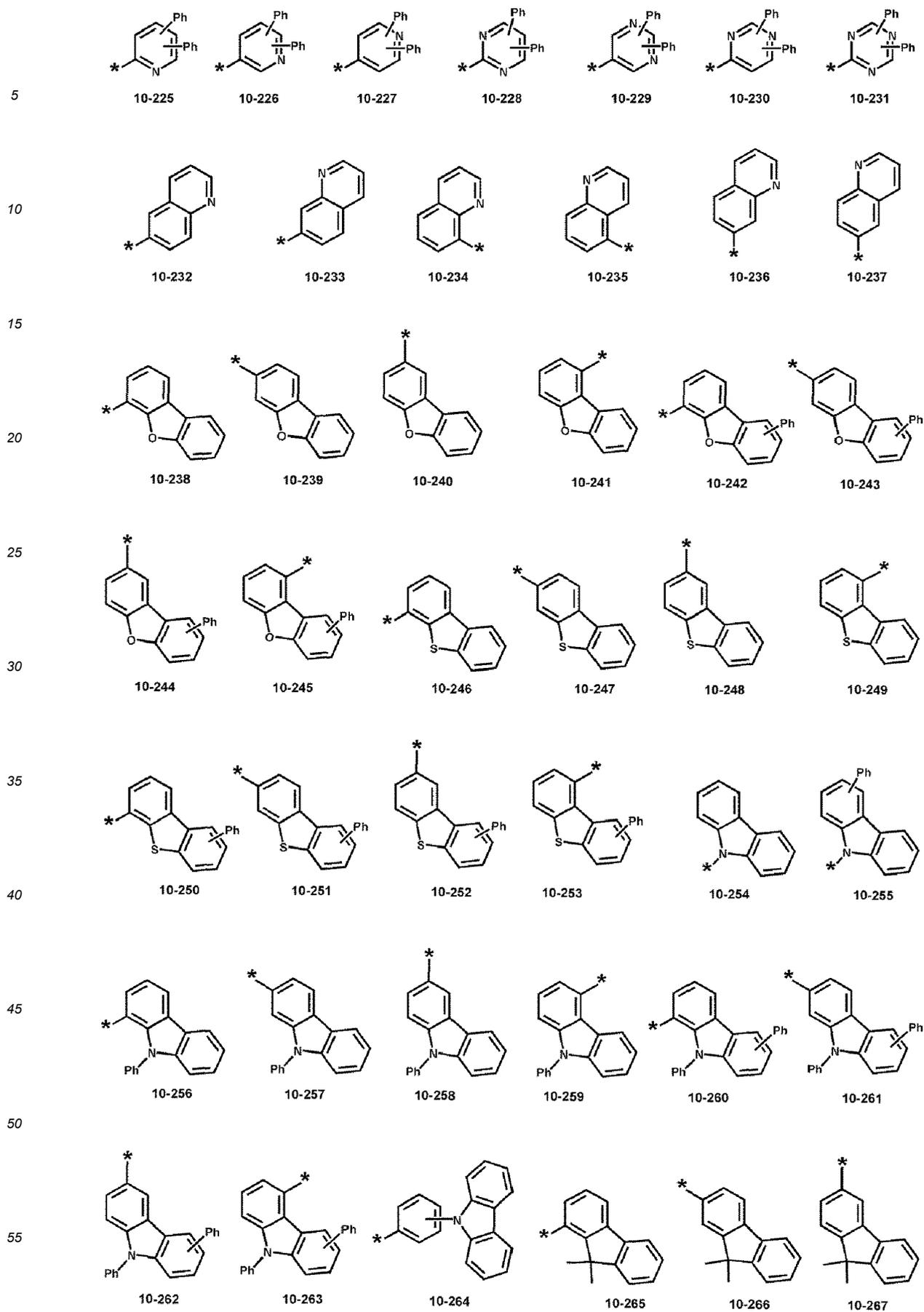
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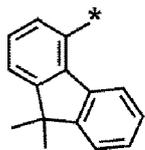
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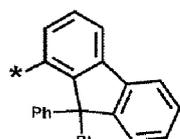
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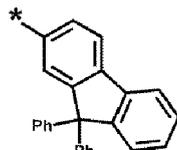
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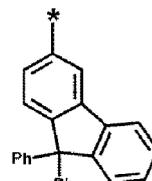
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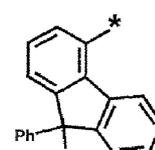
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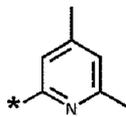


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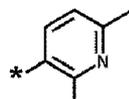


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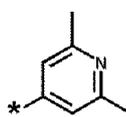
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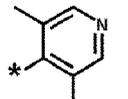
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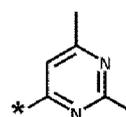
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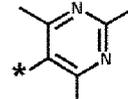
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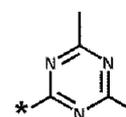
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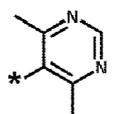
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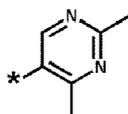
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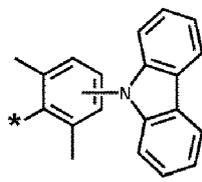
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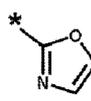


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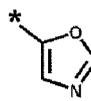


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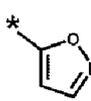
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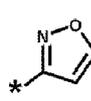
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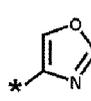
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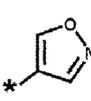
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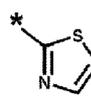
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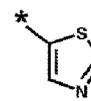
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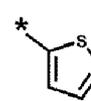
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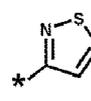


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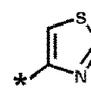


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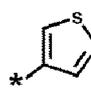
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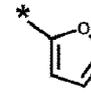
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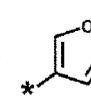
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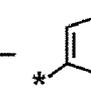
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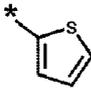
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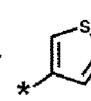
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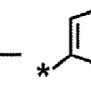
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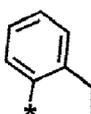
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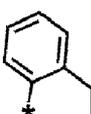
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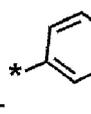
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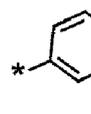
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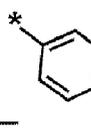
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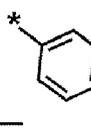
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10-308



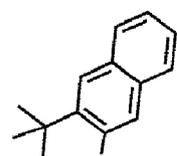
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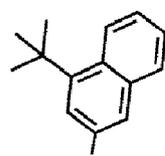
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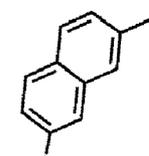
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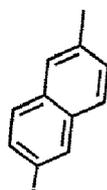
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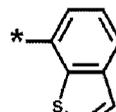
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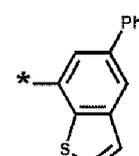
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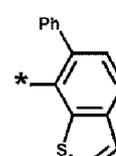
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10-315



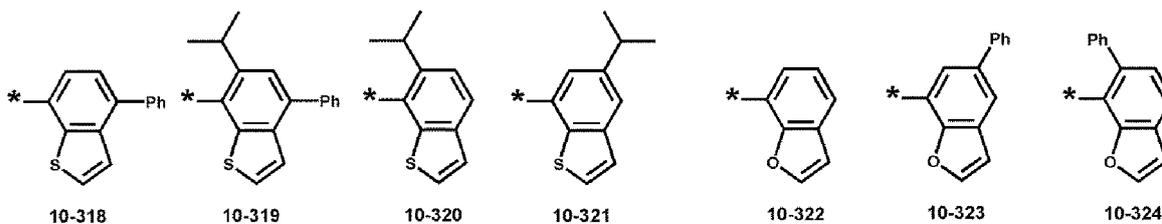
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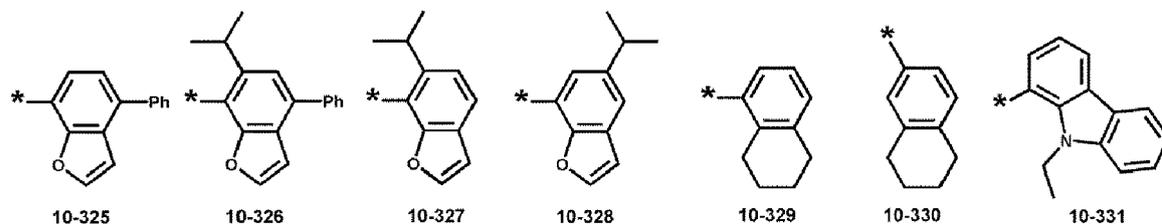
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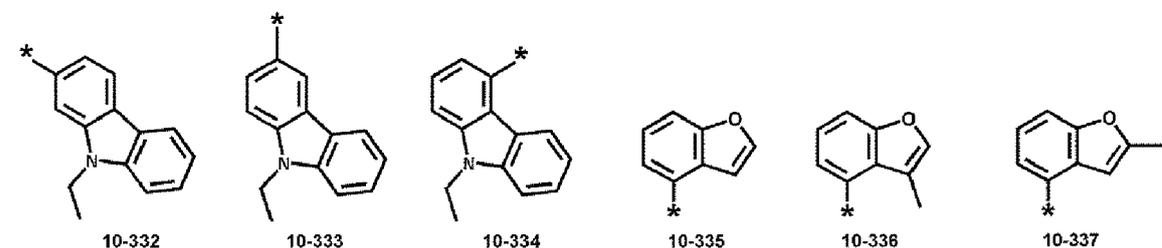


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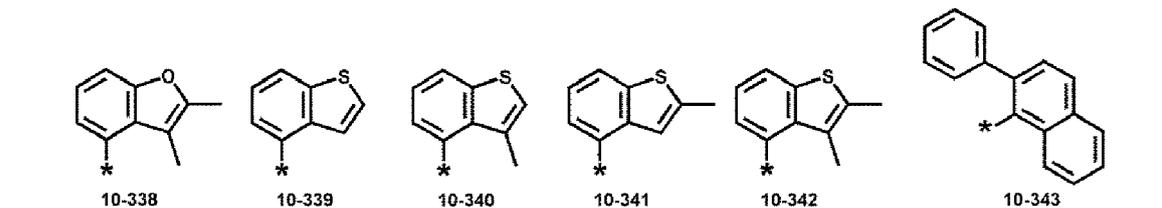
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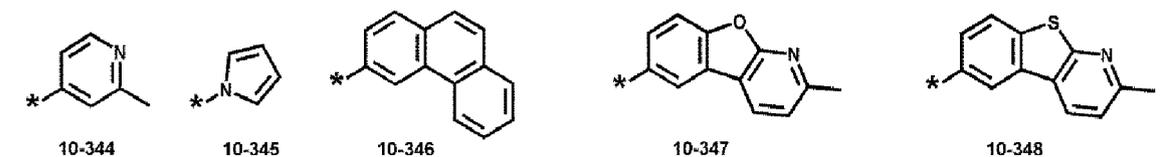
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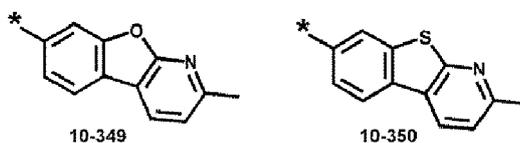


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[0043] In Formulae 9-1 to 9-39, 10-1 to 10-112 and 10-201 to 10-350, * may indicate a binding site to an adjacent atom, "Ph" represents a phenyl group, "TMS" represents a trimethylsilyl group, and "TMG" represents a trimethylgermyl group.

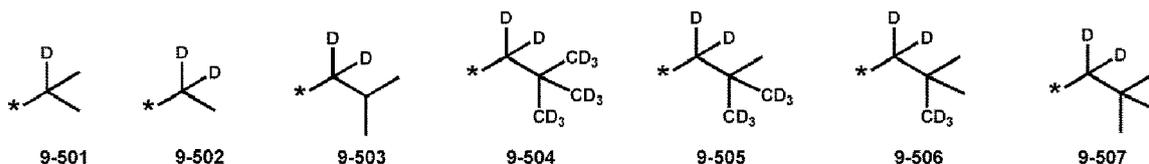
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[0044] The "group represented by Formulae 9-1 to 9-39 in which at least one hydrogen is substituted with deuterium" may be, for example, a group represented by one of Formulae 9-501 to 514:

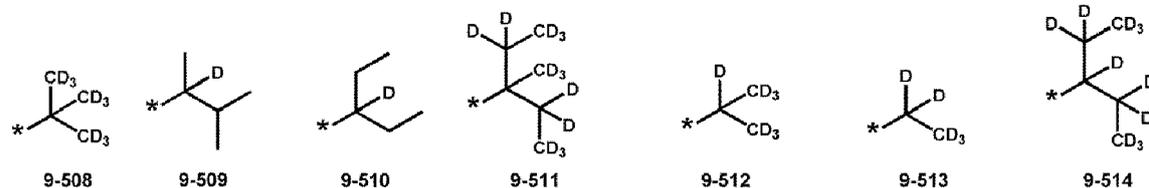
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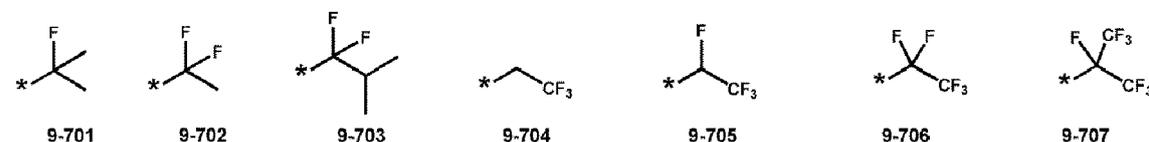
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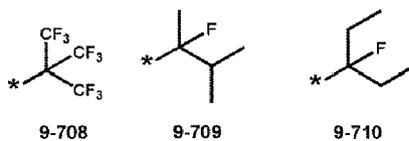
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[0045] The "group represented by Formulae 9-1 to 9-39 in which at least one hydrogen is substituted with -F" may be, for example, a group represented by one of Formulae 9-701 to 710:

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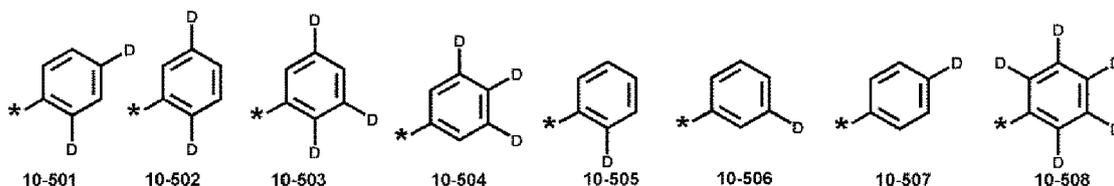
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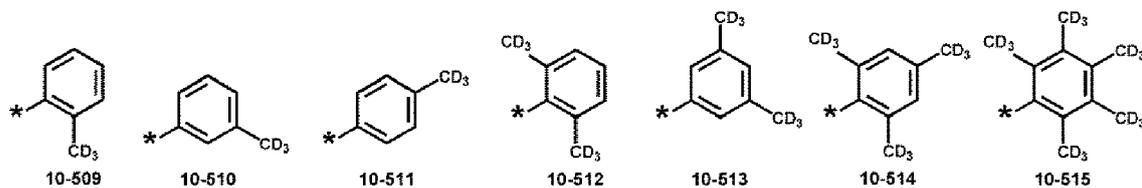
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[0046] The "group represented by Formulae 10-1 to 10-112 in which at least one hydrogen is substituted with deuterium" and the "group represented by Formulae 10-201 to 10-350 in which at least one hydrogen is substituted with deuterium" may each be, for example, a group represented by one of Formulae 10-501 to 553:

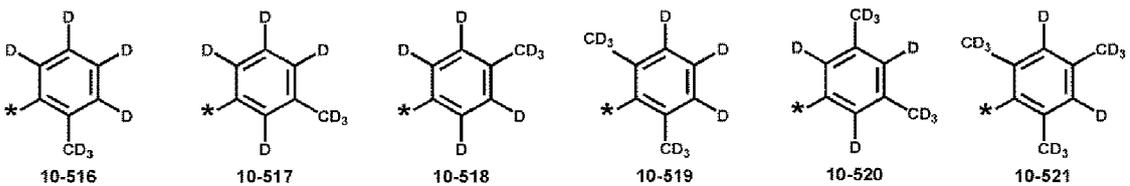
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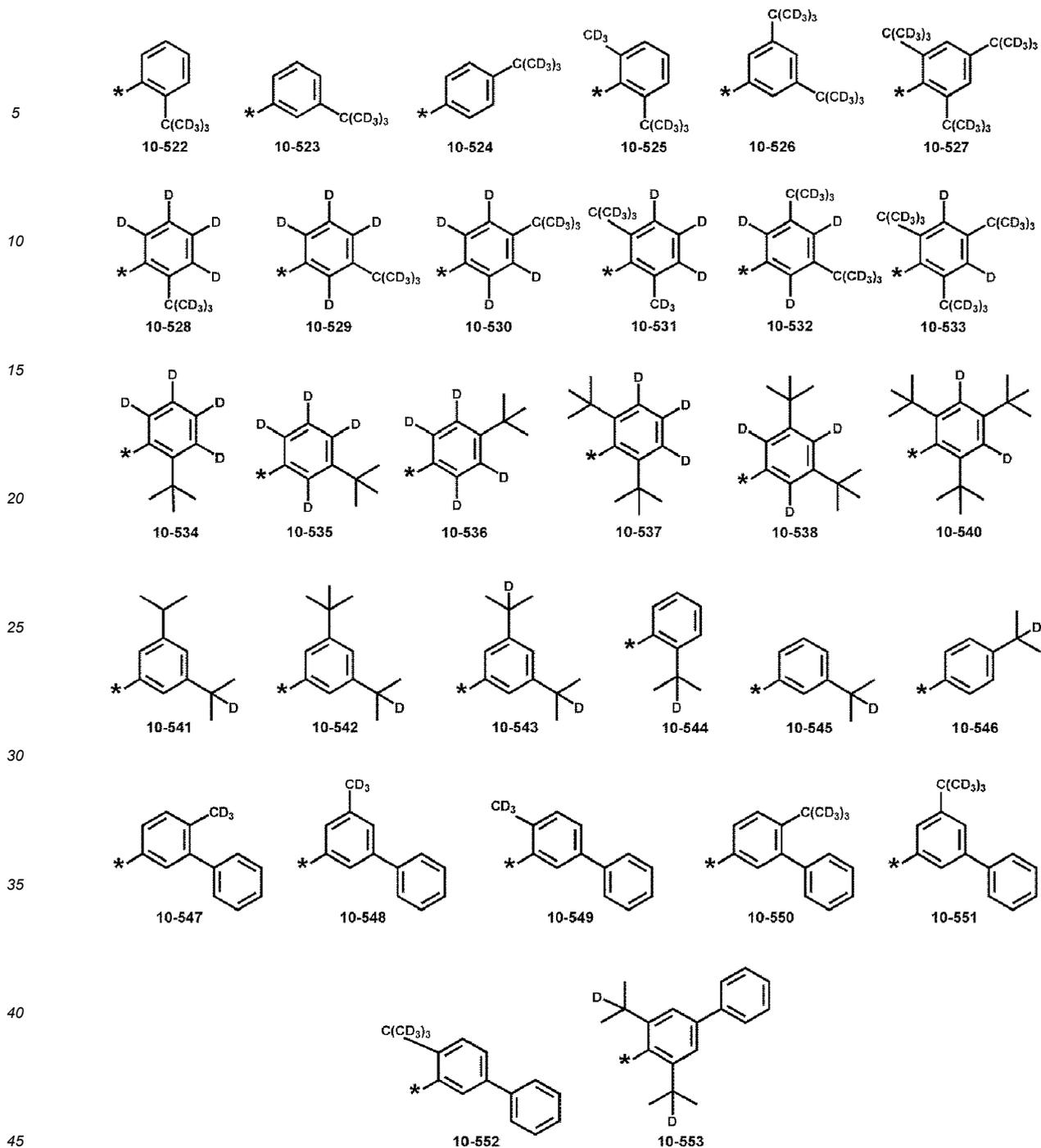
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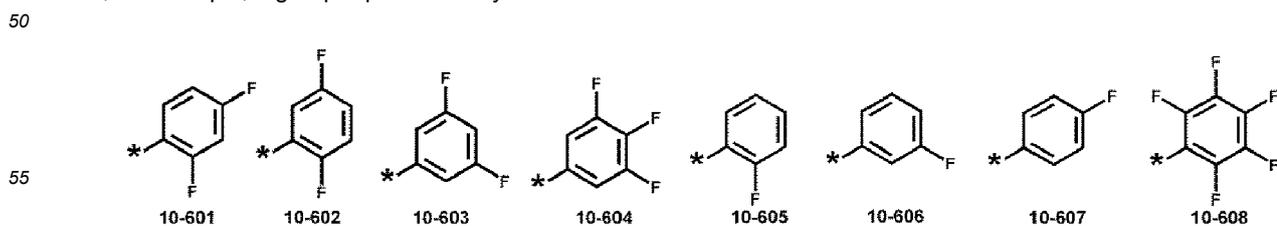
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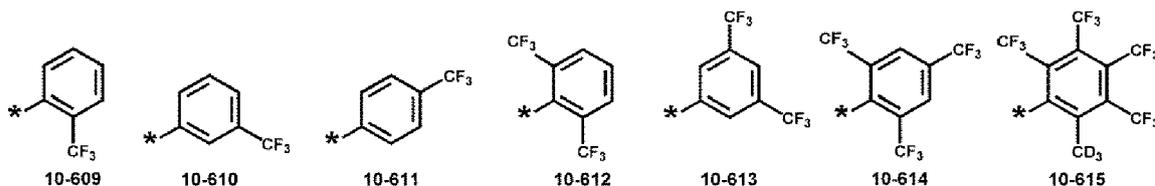
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[0047] The "group represented by Formulae 10-1 to 10-112 in which at least one hydrogen is substituted with -F" and the "group represented by Formulae 10-201 to 10-350 in which at least one hydrogen is substituted with -F" may each be, for example, a group represented by one of Formulae 10-601 to 617:



5



10 [0048] In Formulae 2 and 3, a₁, a₂, and d₁ may respectively indicate the number of R₁(s), R₂(s), and Z₁(s), and a₁, a₂, and d₁ each independently be an integer from 0 to 10. When a₁ is 2 or greater, at least two R₁(s) may be identical to or different from each other, when a₂ is 2 or greater, at least two R₂(s) may be identical to or different from each other, and when d₁ is 2 or greater, at least two Z₁(s) may be identical to or different from each other.

[0049] In some embodiments, a₁, a₂, and d₁ may each independently be 0, 1, 2, 3, 4, 5, or 6.

15 [0050] In Formula 2, the sum of a₁ and a₂ may be 1 or greater. That is, the ligand represented by Formula 2 may be substituted with at least one selected from R₁ and R₂ (in the present specification, R₁ and R₂ may not each be hydrogen).

In some embodiments, the sum of a₁ and a₂ may be an integer from 1 to 5.

[0051] d₂ in Formula 3 may indicate the number of Z₂(s), and d₂ may be an integer from 1 to 10. When d₂ is 2 or greater, at least two Z₂(s) may be identical to or different from each other. That is, ring CY₁₂ in Formula 3 may be substituted with at least one Z₂ (in the present specification, Z₂ may not be hydrogen). In some embodiments, d₂ may be an integer from 1 to 5.

20 [0052] In some embodiments, in Formulae 2 and 3, a₂ and d₂ may each independently be 1, 2, or 3.

[0053] In one or more embodiments, in Formula 2,

- i) a₁ may be 0, and a₂ may be 1 or 2,
- ii) a₁ may be 1 or 2, and a₂ may be 0, or
- iii) a₁ may be 1 or 2, and a₂ may be 1 or 2.

25

[0054] In one or more embodiments, in Formula 3, d₁ may be 0, 1, or 2, and d₂ may be 1, 2, 3, or 4.

[0055] In one or more embodiments, the organometallic compound represented by Formula 1 may include at least one deuterium.

30 [0056] In one or more embodiments, the organometallic compound represented by Formula 1 may include a group represented by -Si(Q₃)(Q₄)(Q₅), a group represented by -Ge(Q₃)(Q₄)(Q₅), or any combination thereof.

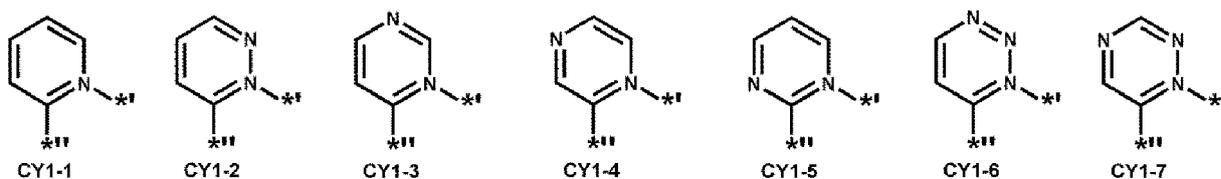
[0057] In Formulae 2 and 3, i) at least two selected from R₁(s) may optionally be linked to each other to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}, ii) at least two selected from R₂(s) may optionally be linked to each other to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}, iii) at least two selected from Z₁(s) may optionally be linked to each other to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}, iv) at least two selected from Z₂(s) may optionally be linked to each other to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}, and v) at least two selected from R₁(s), R₂(s), Z₁(s), and Z₂(s) may optionally be linked to each other to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a}. R_{10a} may be understood by referring to the description of R₁ provided herein.

40 [0058] * and ** in Formulae 2 and 3 may each indicate a binding site to M in Formula 1.

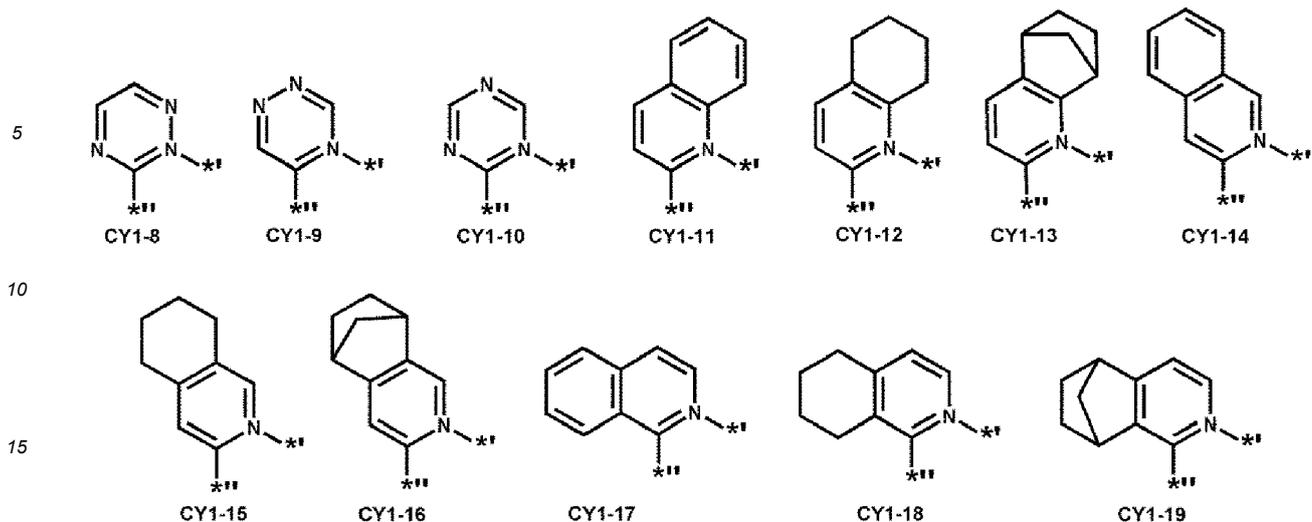
[0059] In some embodiments, in Formulae 2 and 3, the sum of a₁ and d₁ may be 1, 2, or 3.

[0060] In one or more embodiments, ring CY₁ in Formula 2 may be a group represented by one of Formulae CY1-1 to CY1-19:

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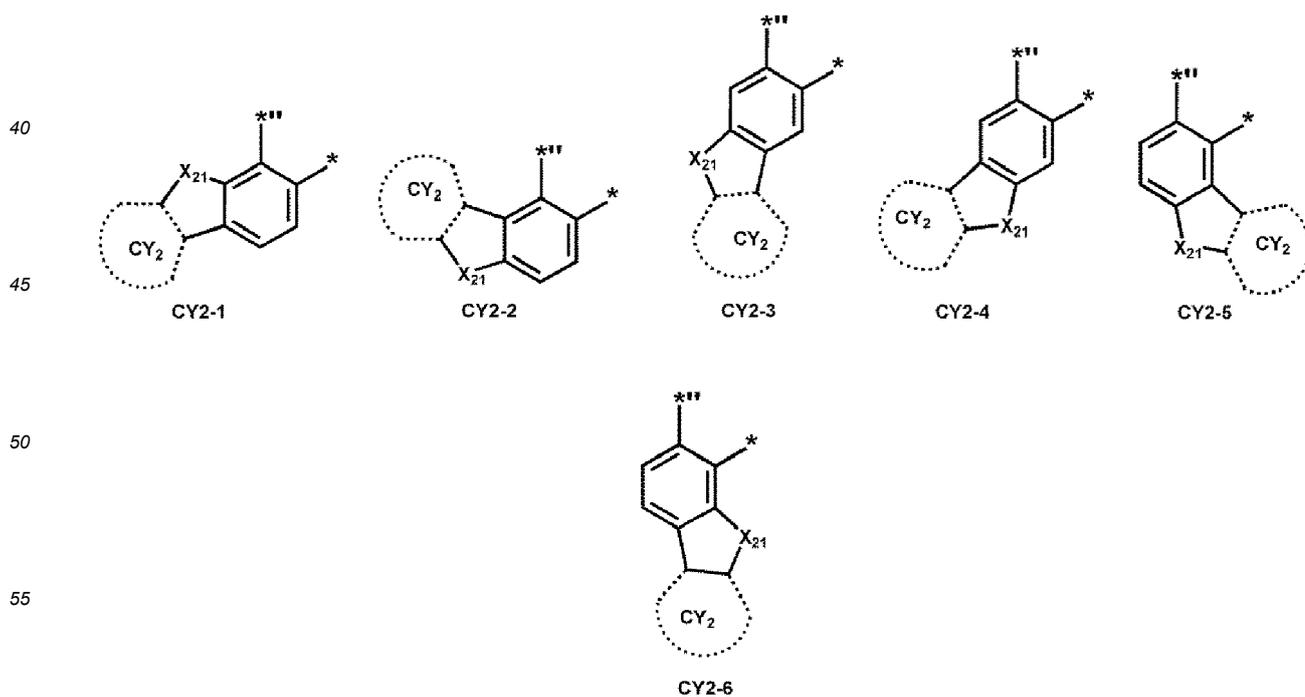


20 **[0061]** In Formulae CY1-1 to CY1-19, * may indicate a binding site to M in Formula 1, and ** may indicate a binding site to an adjacent benzo group.

[0062] In one or more embodiments, a group represented by



35 in Formula 2 may be a group represented by one of Formulae CY2-1 to CY2-6:

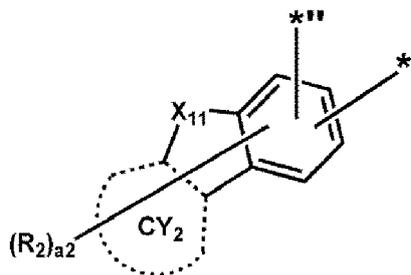


[0063] In Formulae CY2-1 to CY2-6, X₂₁ and ring CY₂ may each be understood by referring to the descriptions thereof provided herein, * may indicate a binding site to M in Formula 1, and *** may indicate a binding site to ring CY₁ in Formula 2.

[0064] In one or more embodiments, a group represented by

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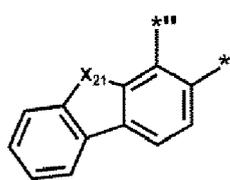
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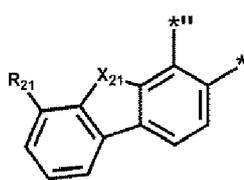
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in Formula 2 may be a group represented by one of Formulae CY2(1) to CY2(22):

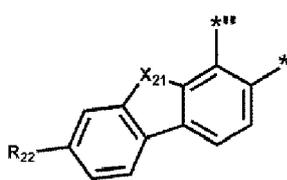
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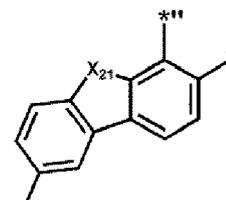
CY2(1)



CY2(2)

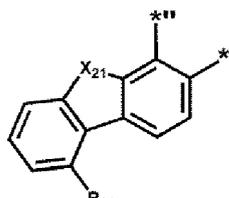


CY2(3)

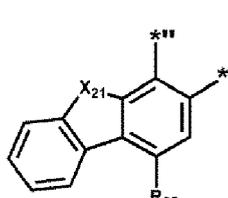


CY2(4)

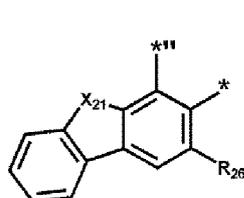
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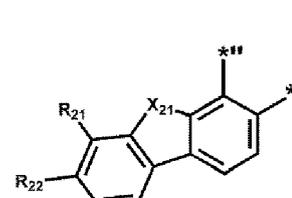
CY2(5)



CY2(6)

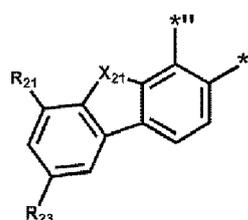


CY2(7)

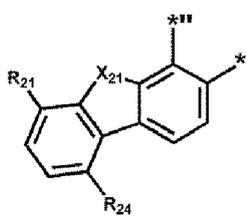


CY2(8)

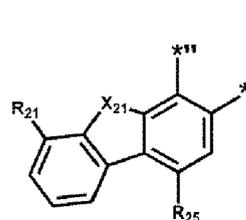
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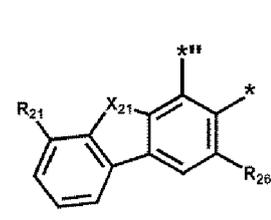
CY2(9)



CY2(10)



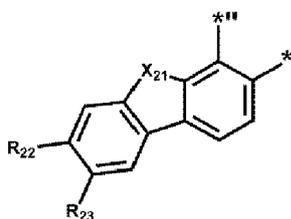
CY2(11)



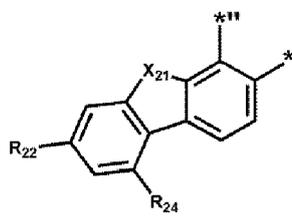
CY2(12)

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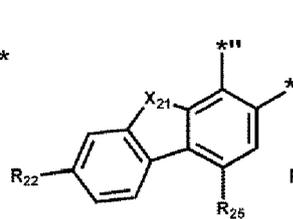
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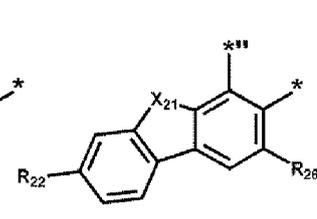
CY2(13)



CY2(14)

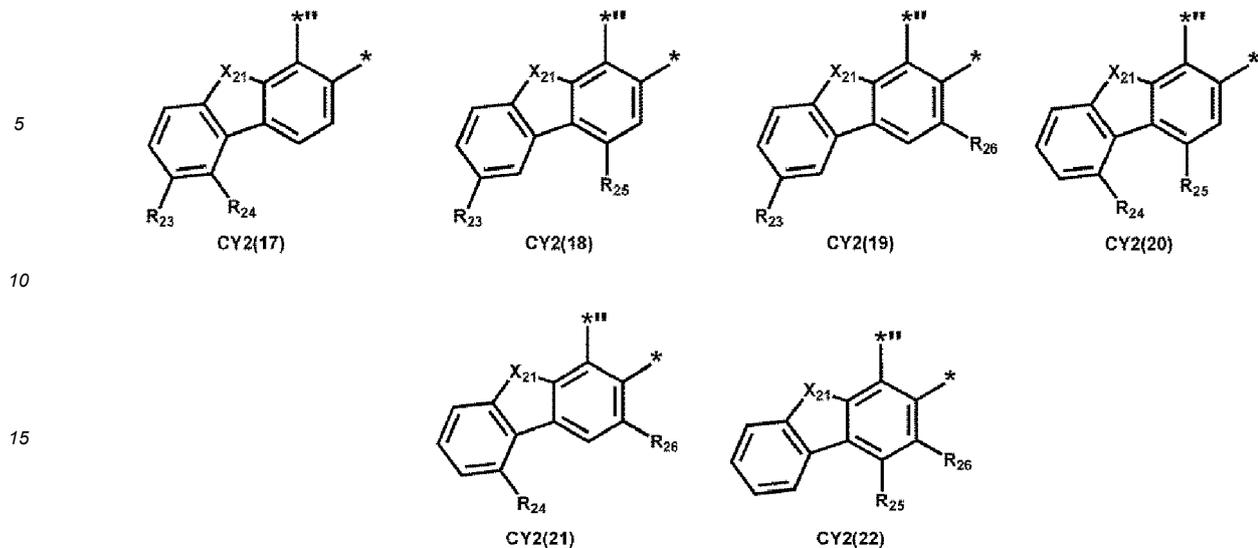


CY2(15)



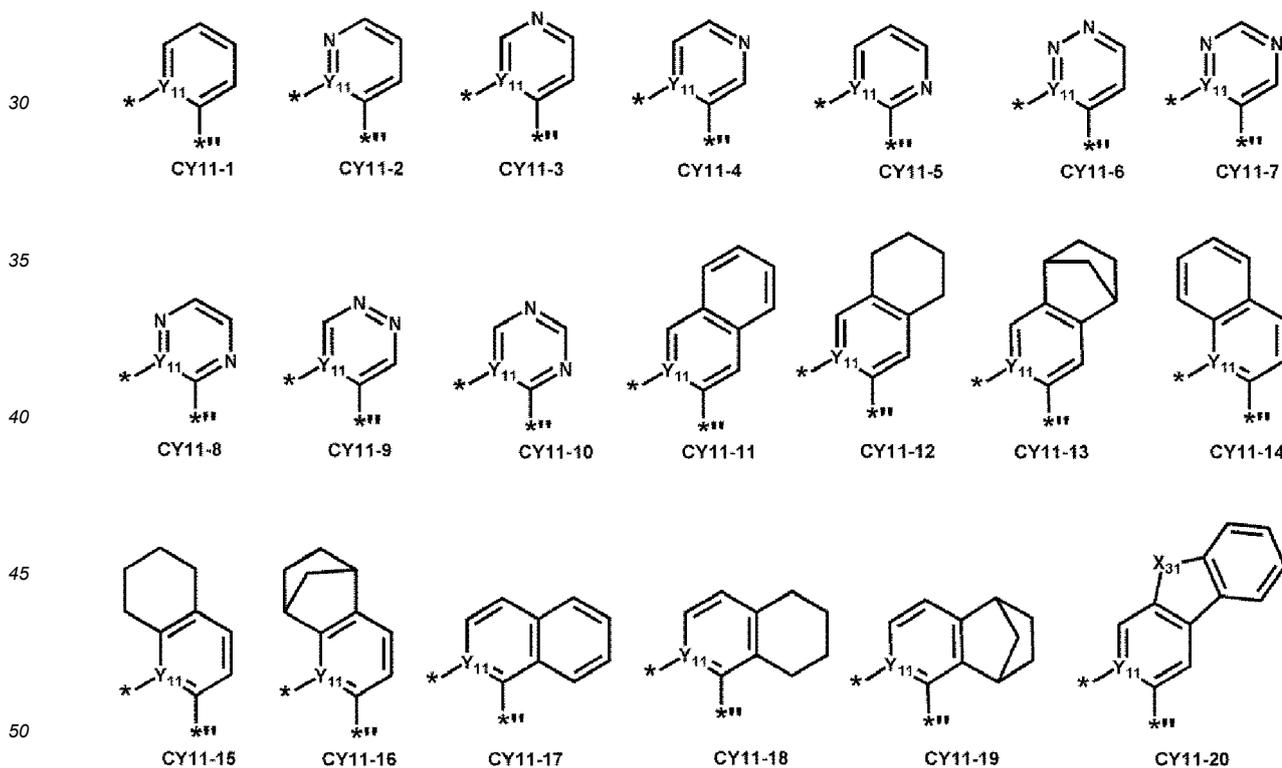
CY2(16)

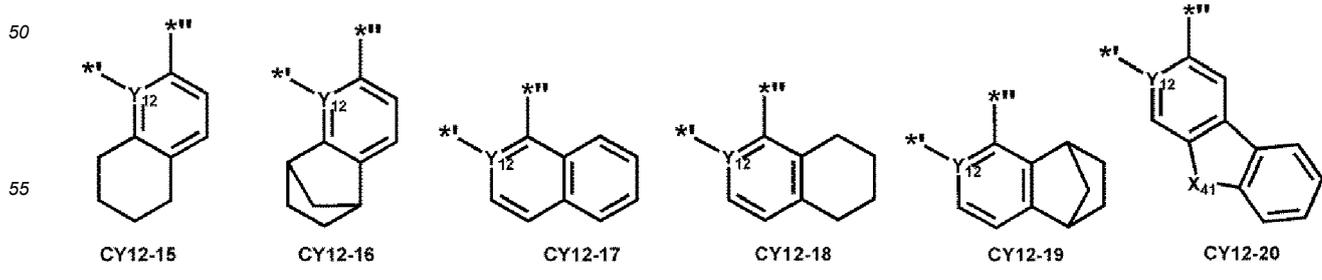
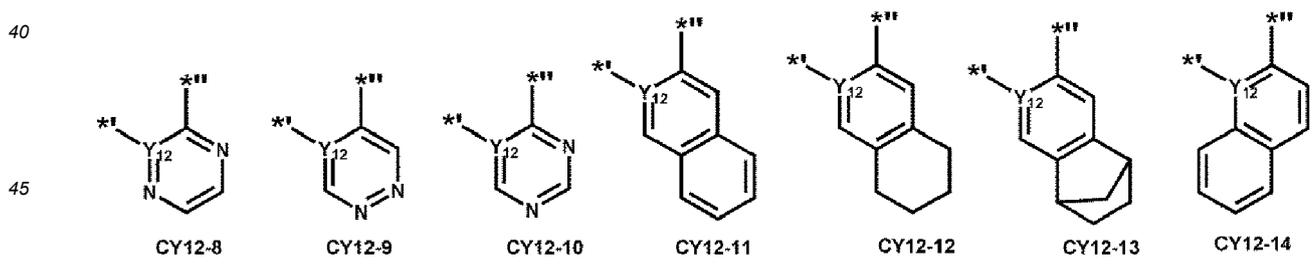
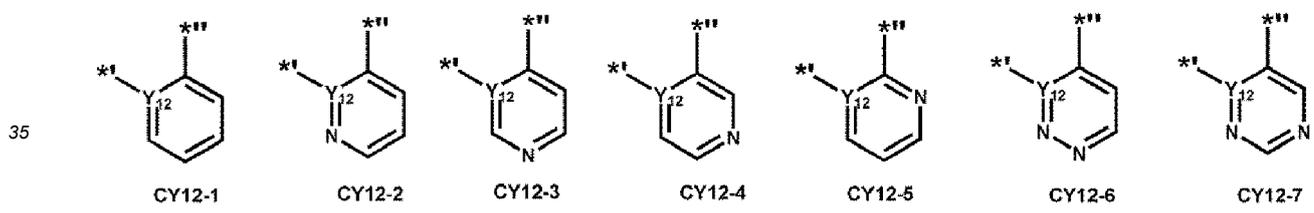
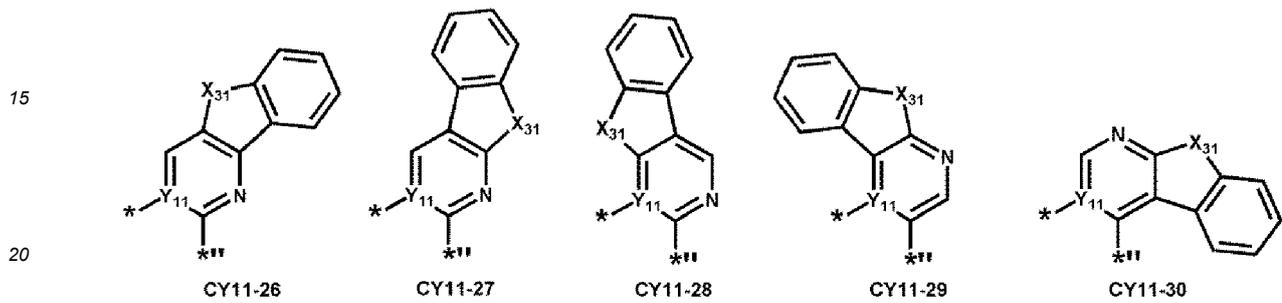
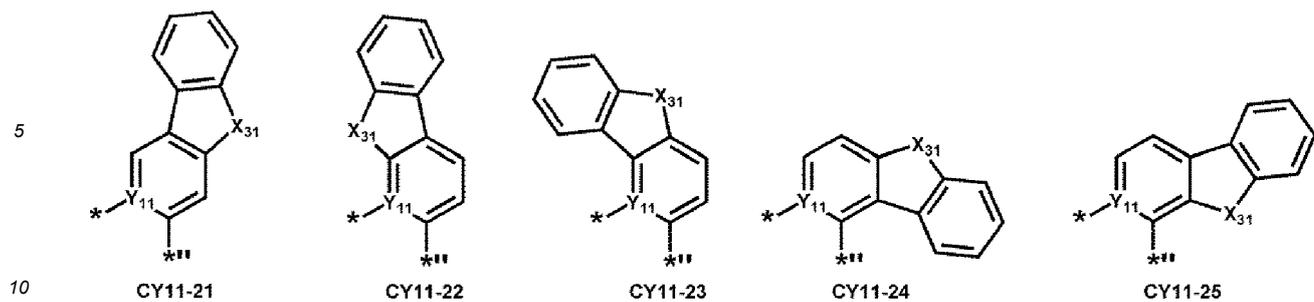
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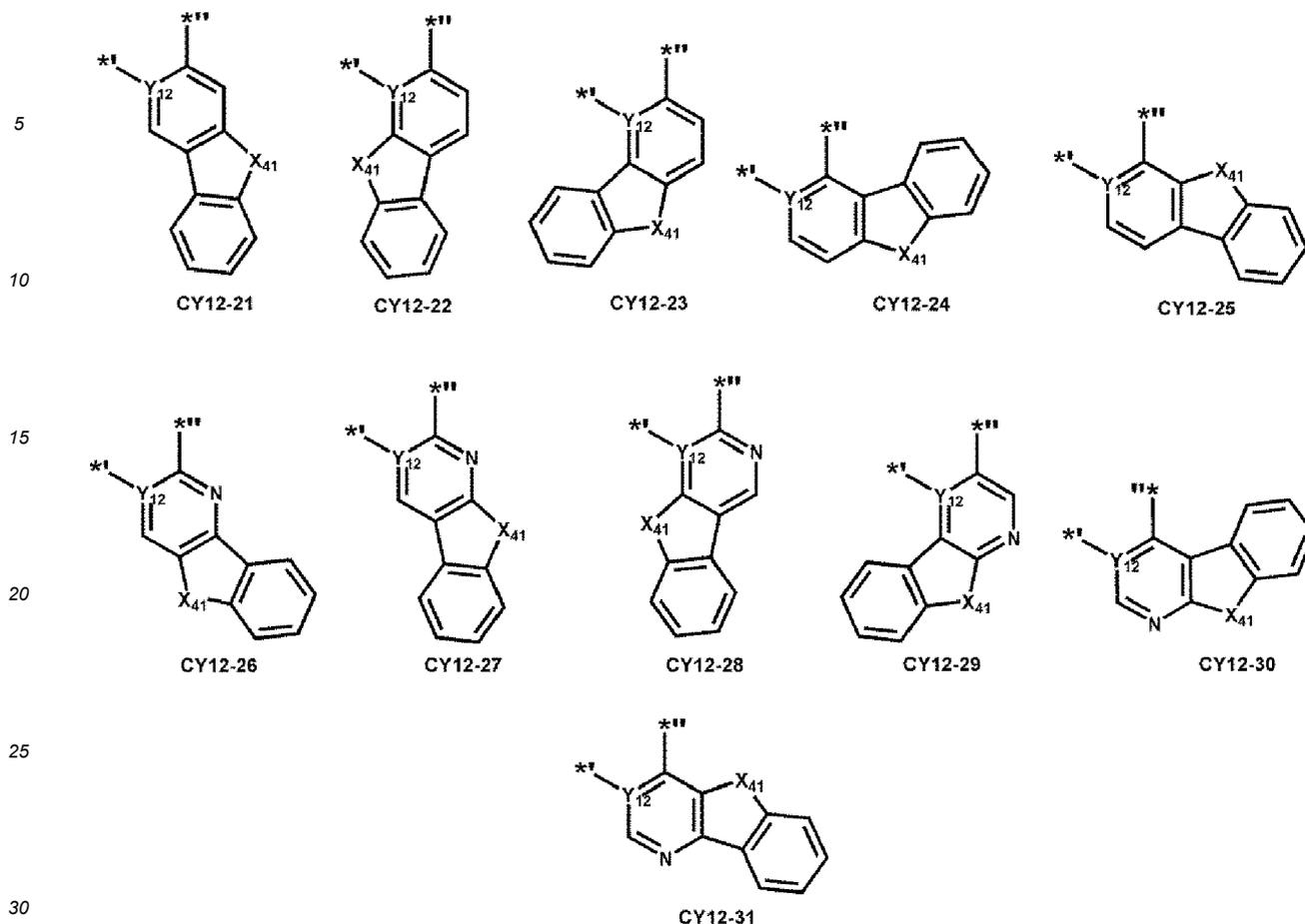


[0065] In Formulae CY2(1) to CY2(22), X₂₁ may be understood by referring to the description thereof provided herein, R₂₁ to R₂₆ may each be understood by referring to the description of R₂ provided herein, * may indicate a binding site to M in Formula 1, and ** may indicate a binding site to ring CY1 in Formula 2.

[0066] In one or more embodiments, ring CY₁₁ in Formula 3 may be a group represented by one of Formulae CY11-1 to CY11-31, and/or ring CY₁₂ in Formula 3 may be a group represented by one of Formulae CY12-1 to CY12-31:







[0067] In Formulae CY11-1 to CY11-31 and CY12-1 to CY12-31,

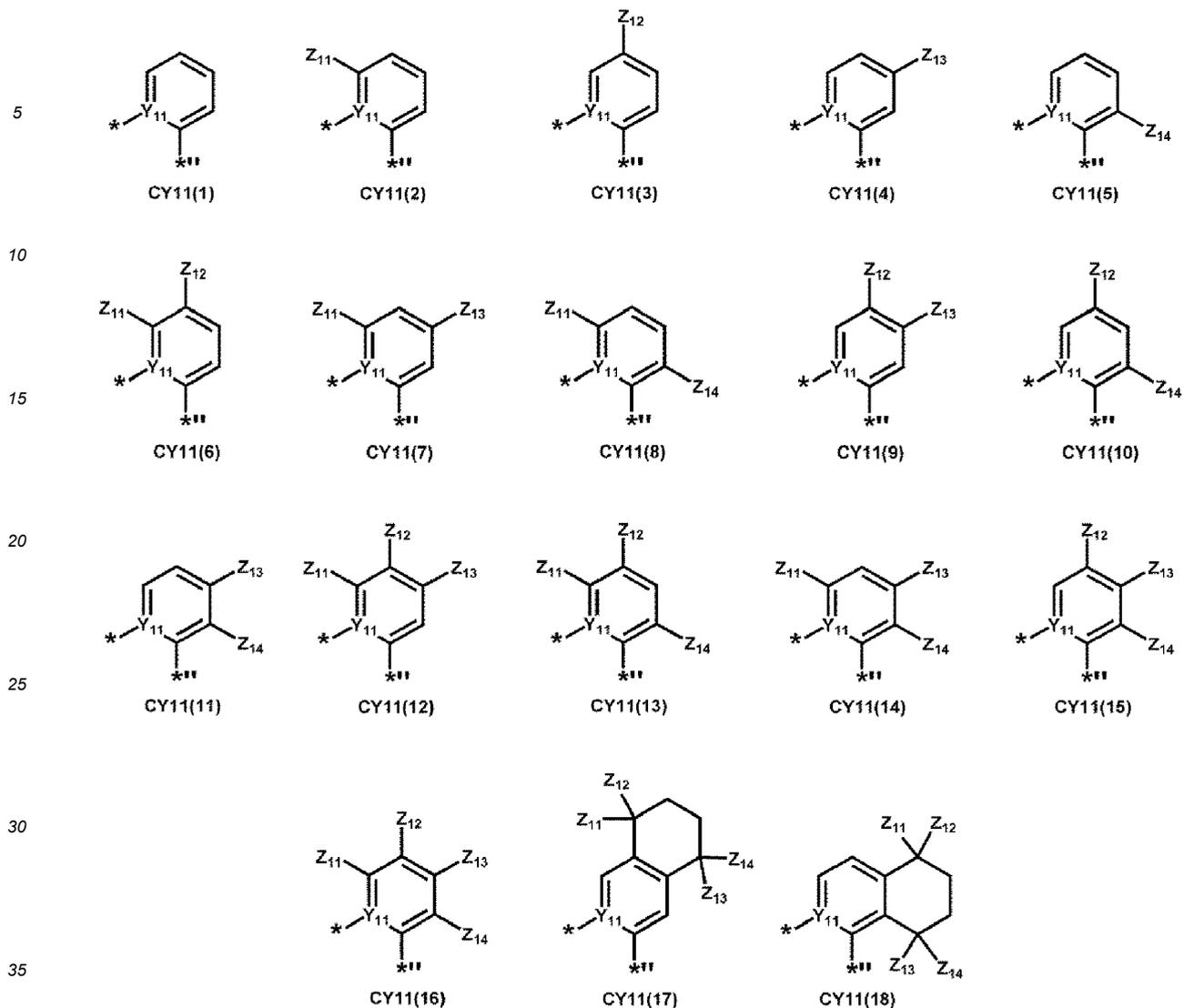
35 Y_{11} and Y_{12} may respectively be understood by referring to the descriptions of Y_{11} and Y_{12} provided herein,
 X_{31} may be O, S, N(Z_{18}), C(Z_{18})(Z_{19}), or Si(Z_{18})(Z_{19}),
 X_{41} may be O, S, N(Z_{28}), C(Z_{28})(Z_{29}), or Si(Z_{28})(Z_{29}),
 Z_{18} and Z_{19} may each be understood by referring to the descriptions of Z_1 provided herein,
 Z_{28} and Z_{29} may each be understood by referring to the descriptions of Z_2 provided herein,
 40 * and *' in Formulae CY11-1 to CY11-31 and CY12-1 to CY12-31 may each indicate a binding site to M in Formula 1, and *** indicates a binding site to an adjacent atom in Formula 3.

[0068] In one or more embodiments, a group represented by



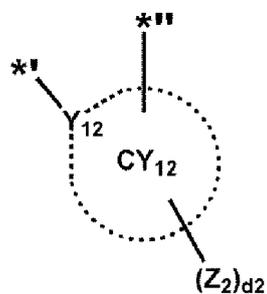
in Formula 3 may be a group represented by one of Formulae CY11(1) to CY11(18):

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[0069] In Formulae CY11(1) to CY11(18), Y_{12} may be understood by referring to the description thereof provided herein, Z_{11} to Z_{14} may each be understood by referring to the description of Z_1 provided herein, * may indicate a binding site to M in Formula 1, and *** may indicate a binding site to an adjacent atom in Formula 3.

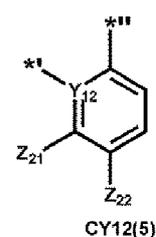
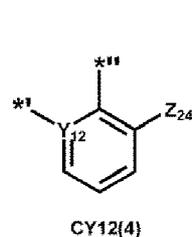
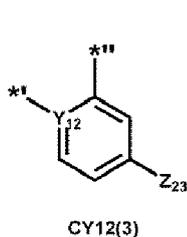
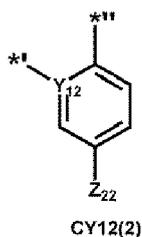
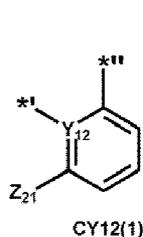
[0070] In one or more embodiments, a group represented by



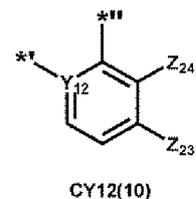
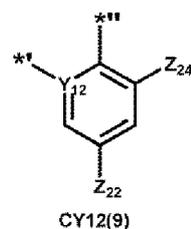
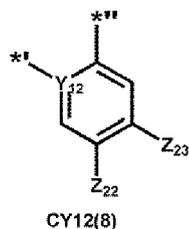
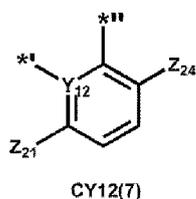
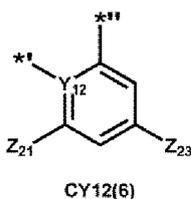
in Formula 3 may be a group represented by one of Formulae CY12(1) to CY12(17):

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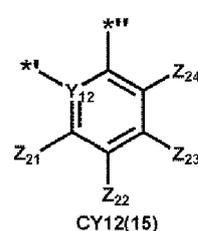
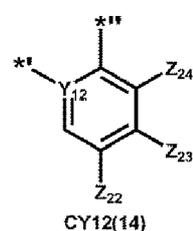
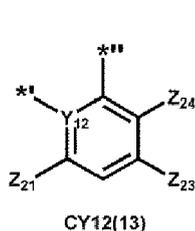
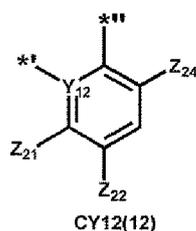
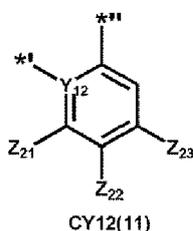


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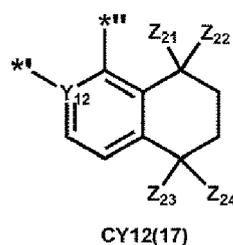
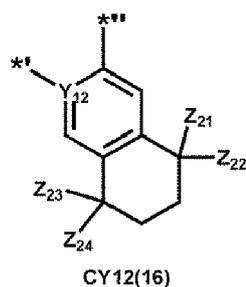
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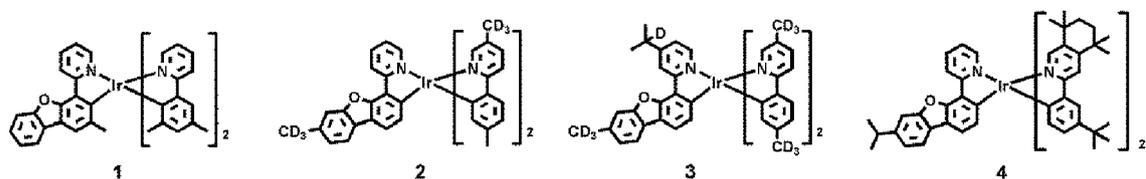
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[0071] In Formulae CY12(1) to CY12(17), Y_{12} may be understood by referring to the description thereof provided herein, Z_{21} to Z_{24} may each be understood by referring to the description of Z_2 provided herein, * may indicate a binding site to M in Formula 1, and *** may indicate a binding site to an adjacent atom in Formula 3.

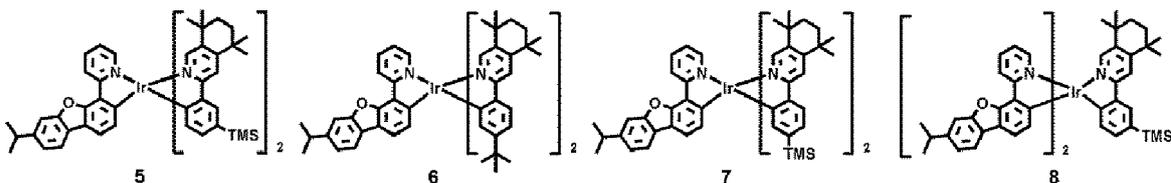
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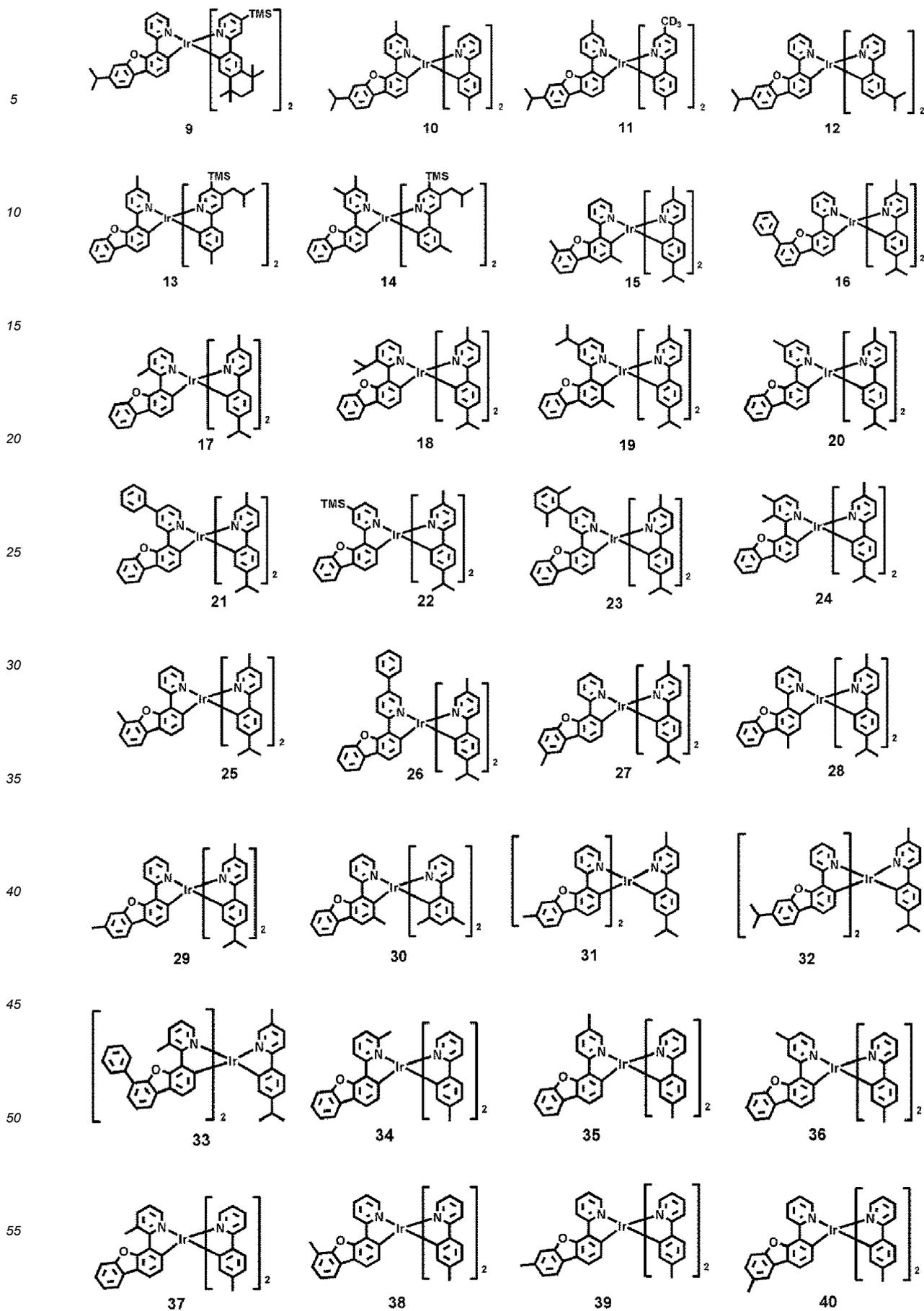
[0072] In one or more embodiments, the organometallic compound represented by Formula 1 may be of Compounds 1 to 296:

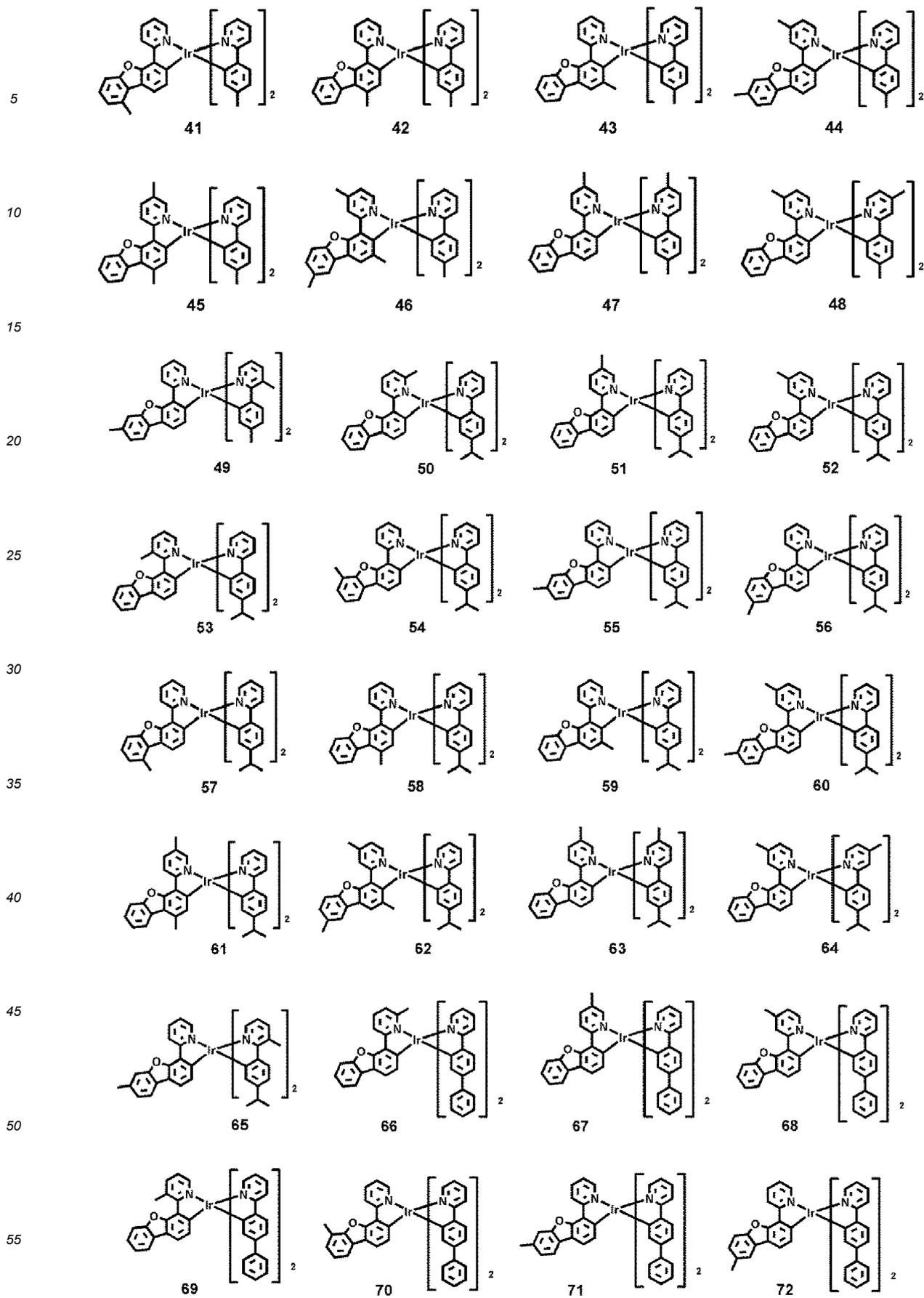
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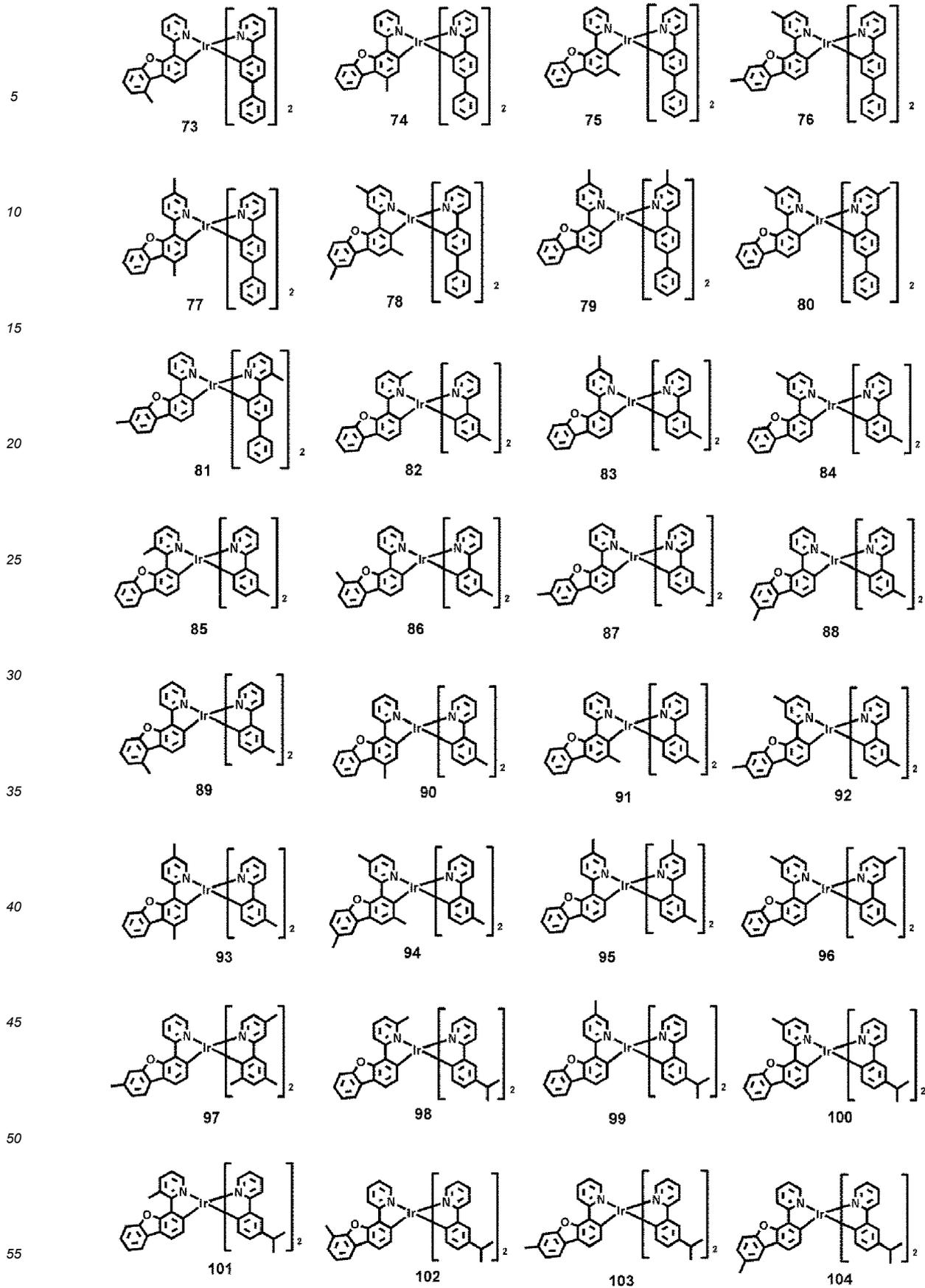


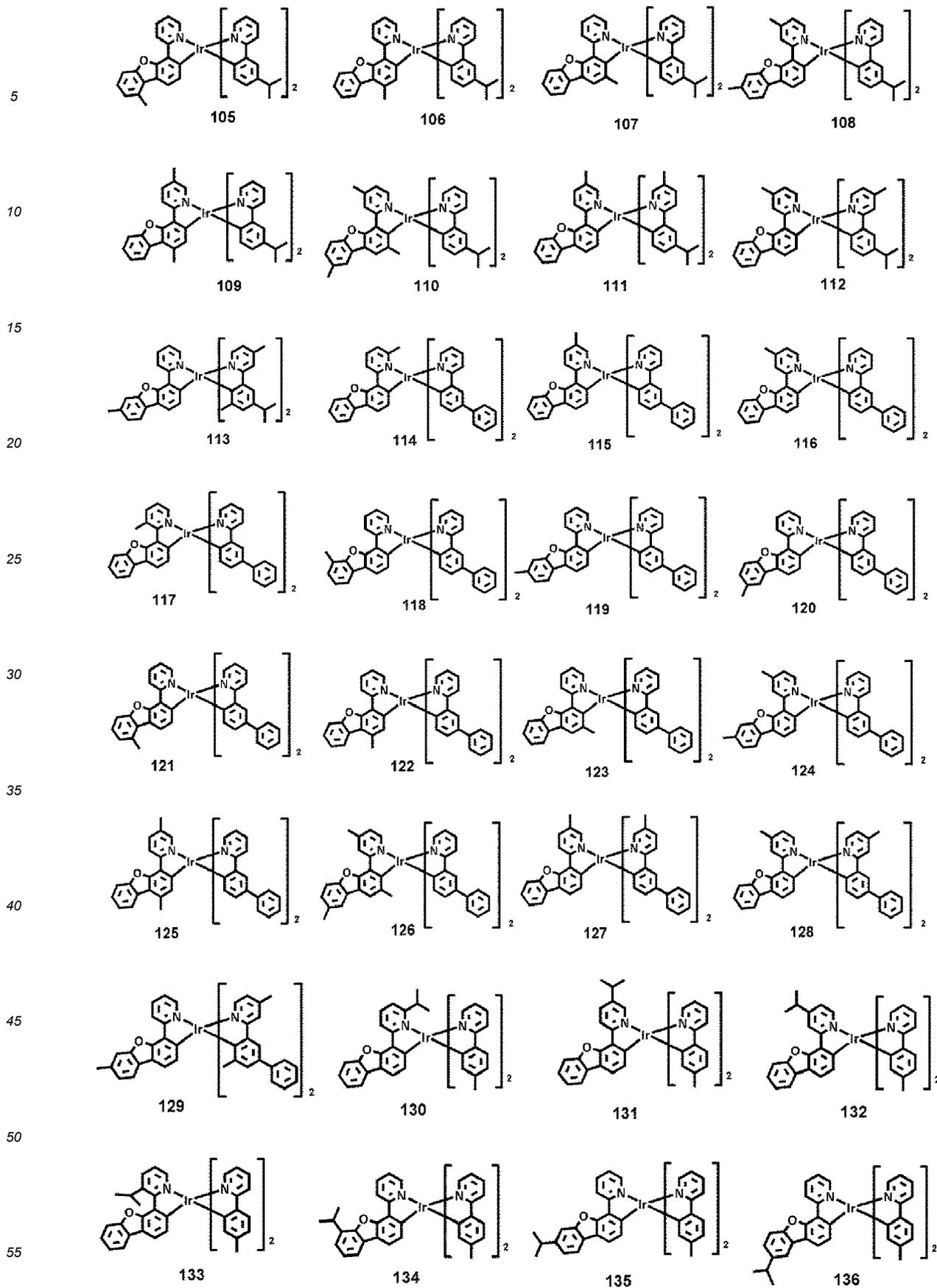
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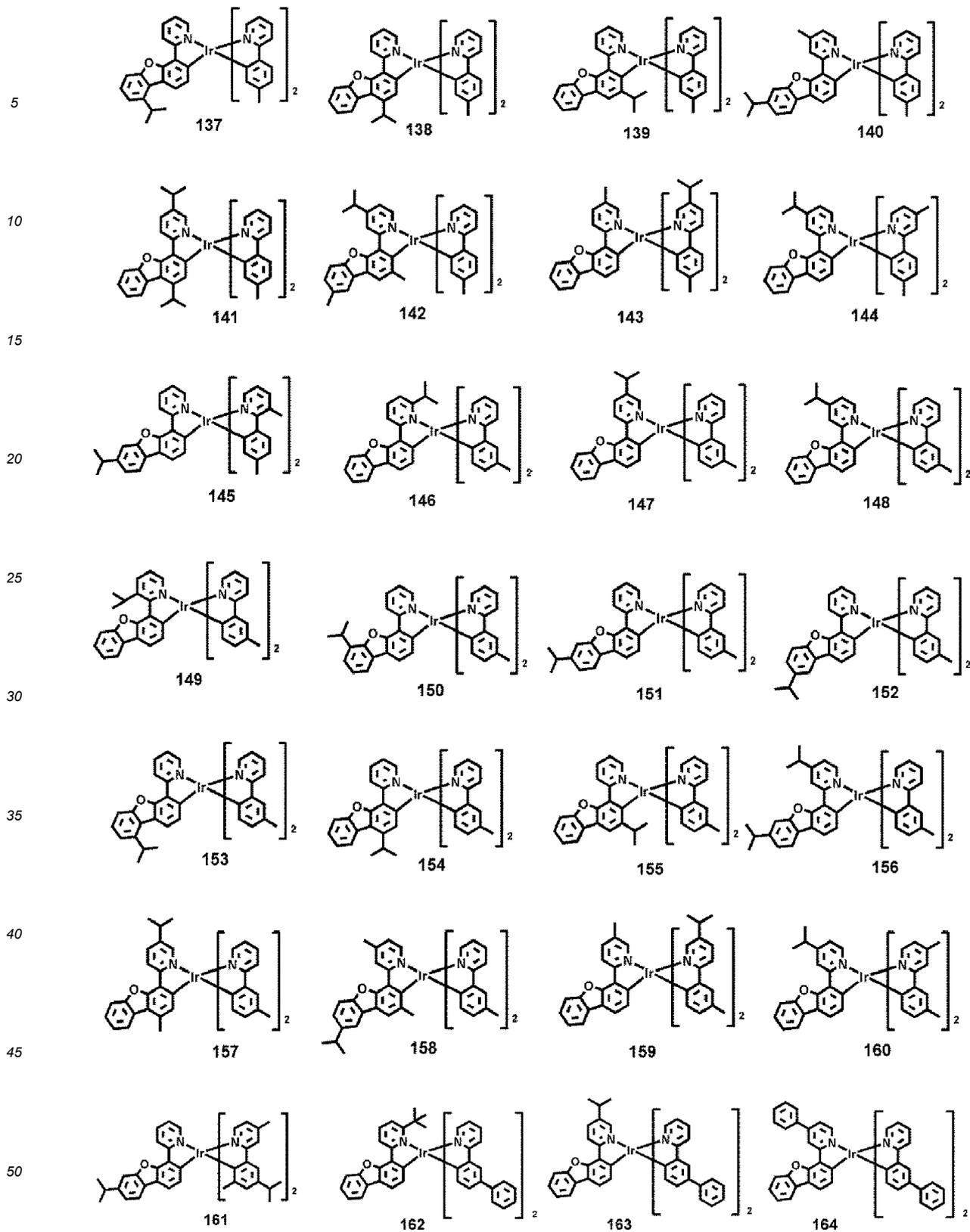


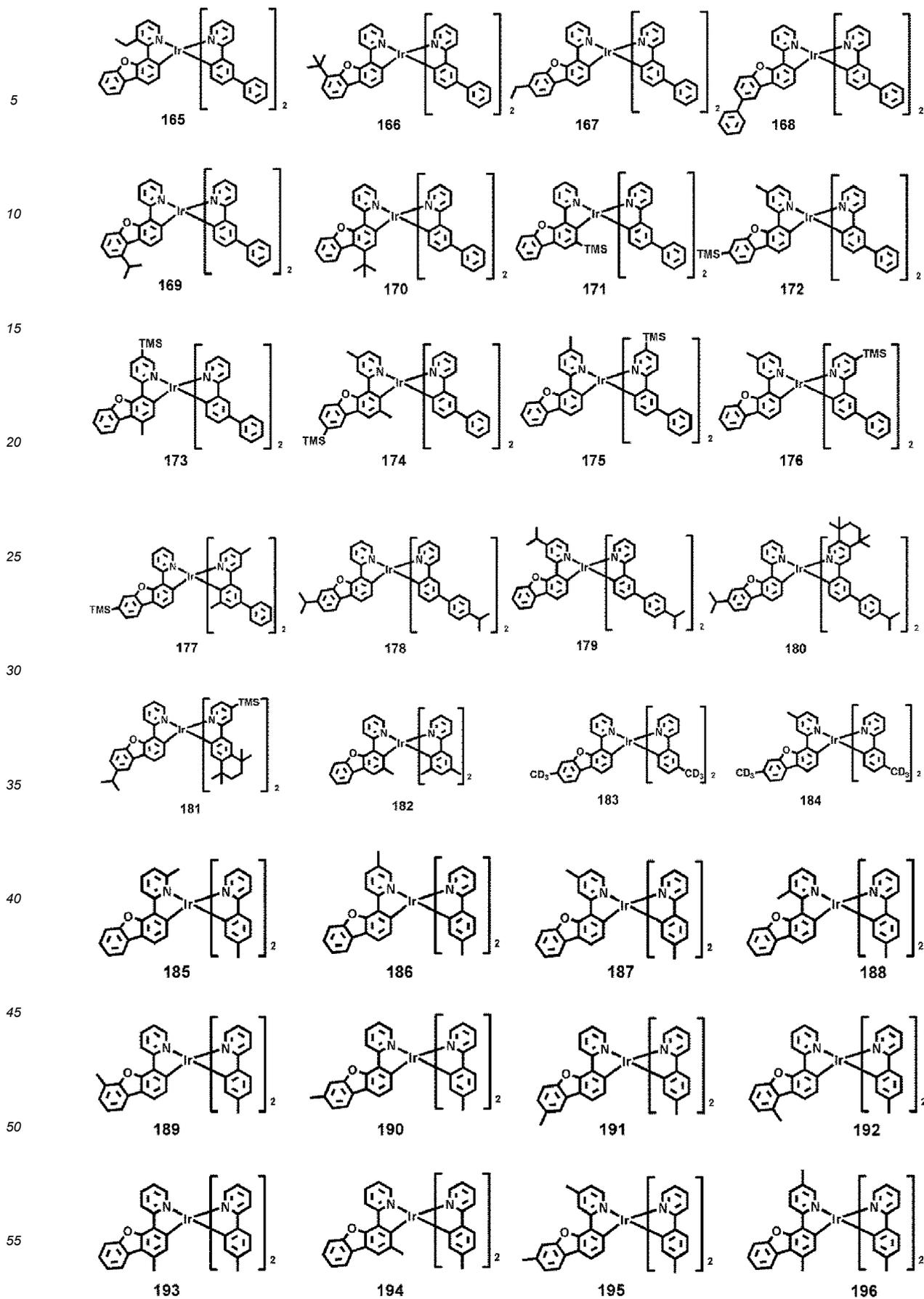




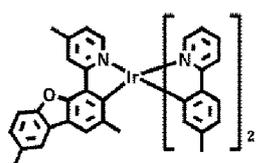




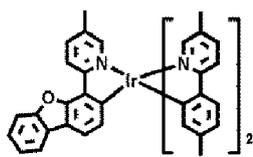




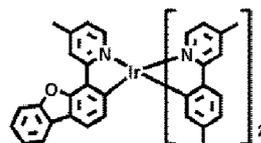
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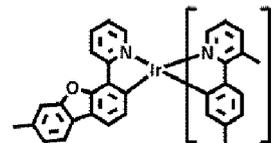
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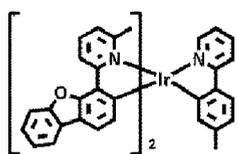


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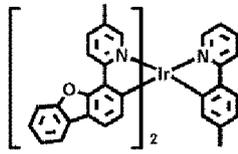


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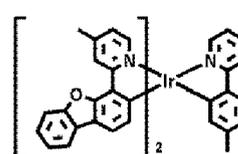
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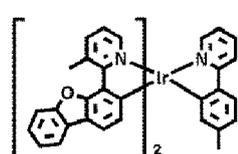
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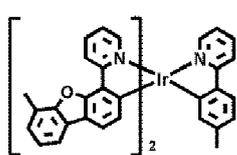


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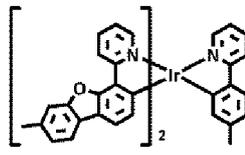


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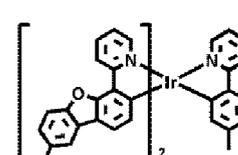
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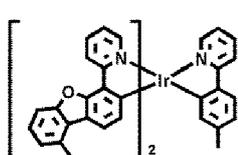
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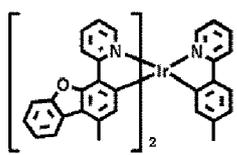


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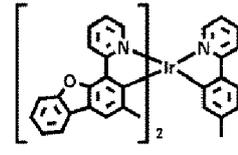


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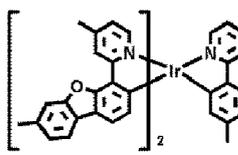
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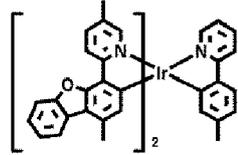
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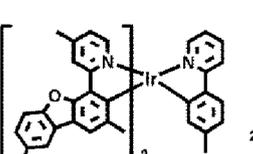


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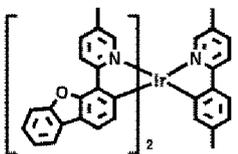


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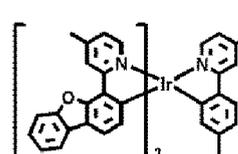
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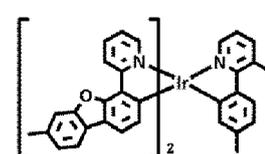
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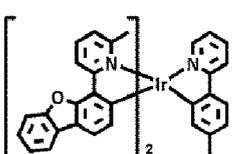


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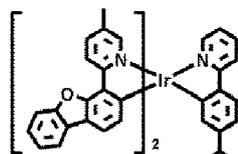


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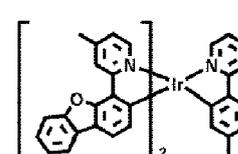
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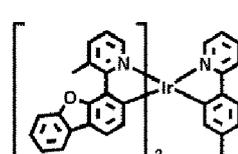
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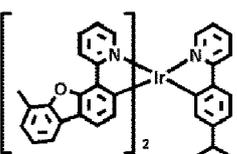


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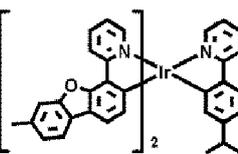


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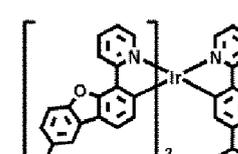
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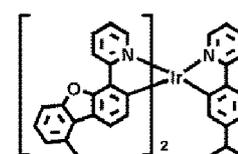
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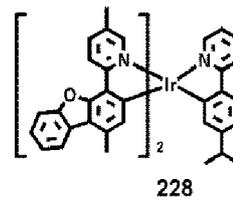
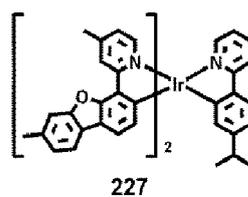
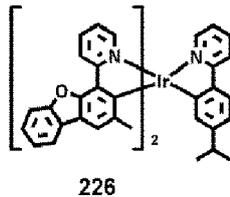
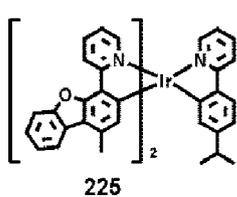


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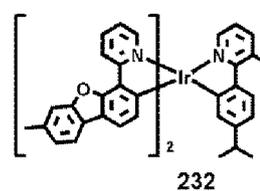
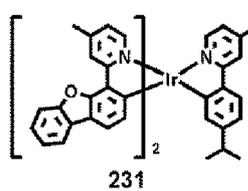
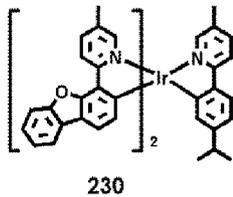
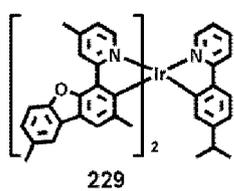
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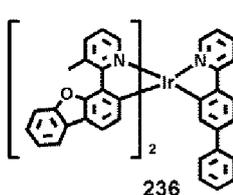
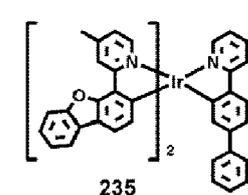
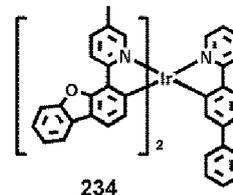
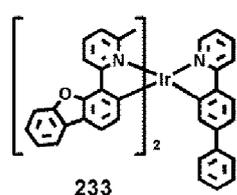
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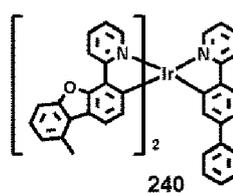
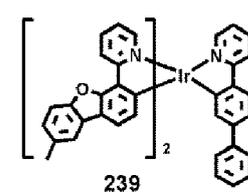
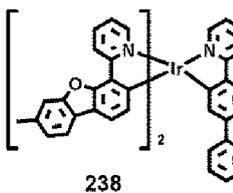
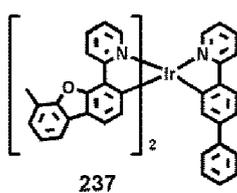
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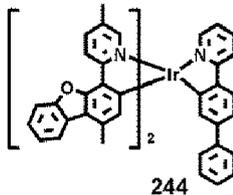
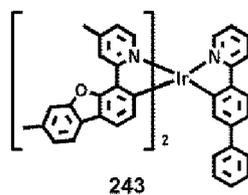
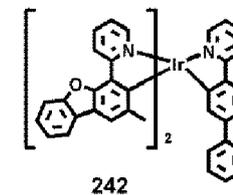
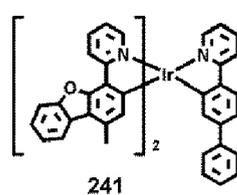


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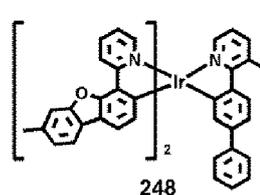
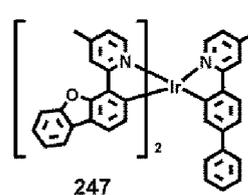
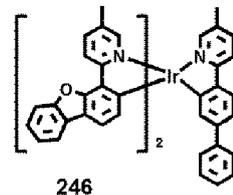
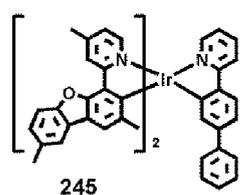
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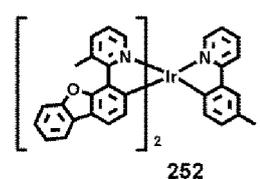
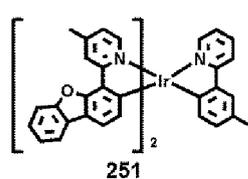
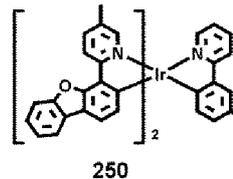
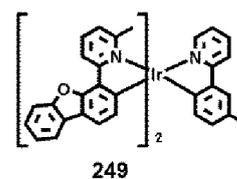
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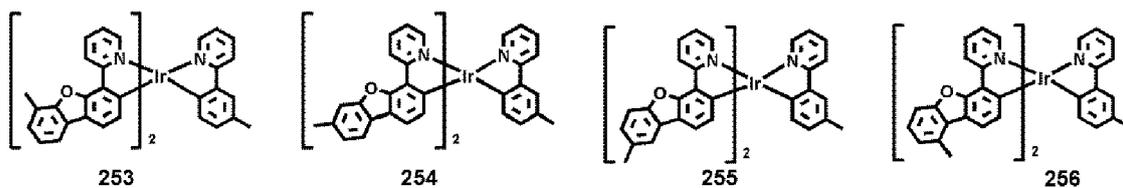
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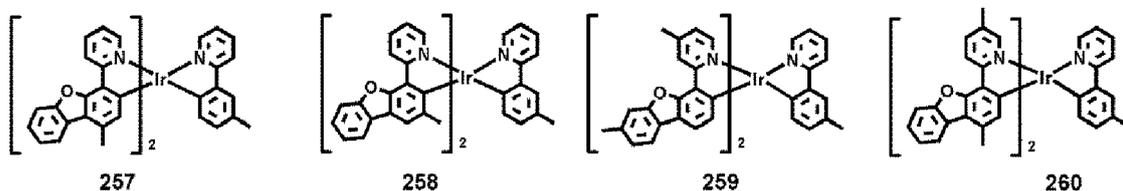


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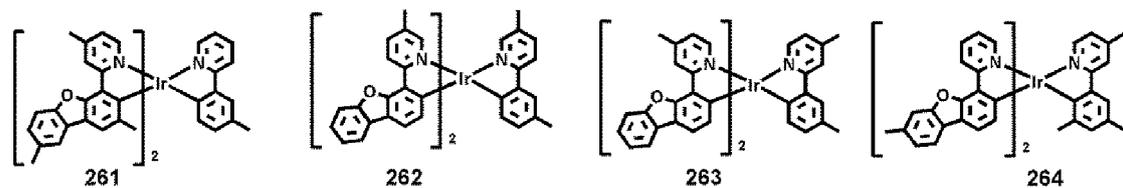
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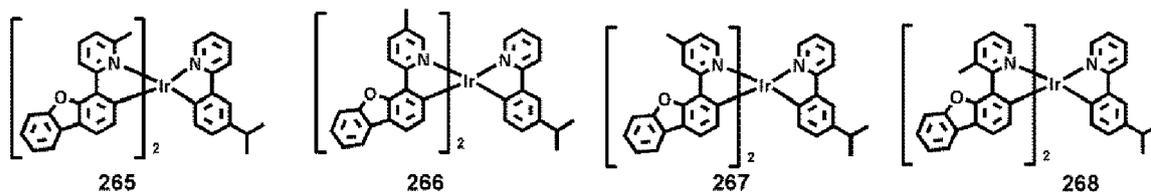
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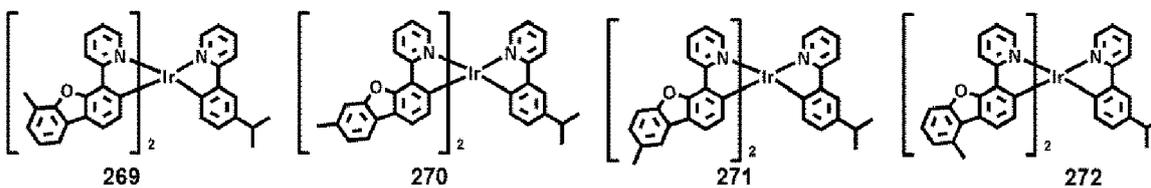


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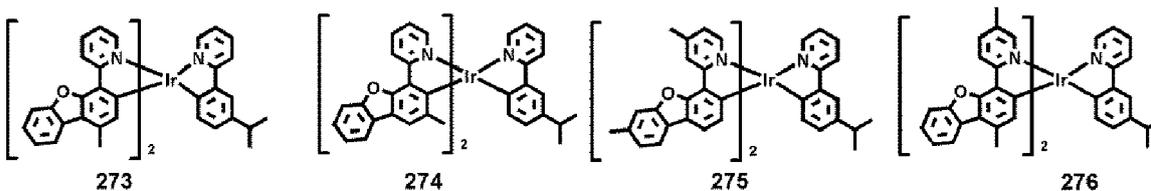
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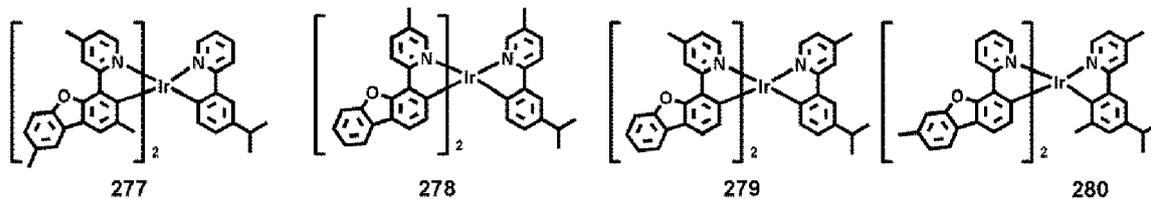
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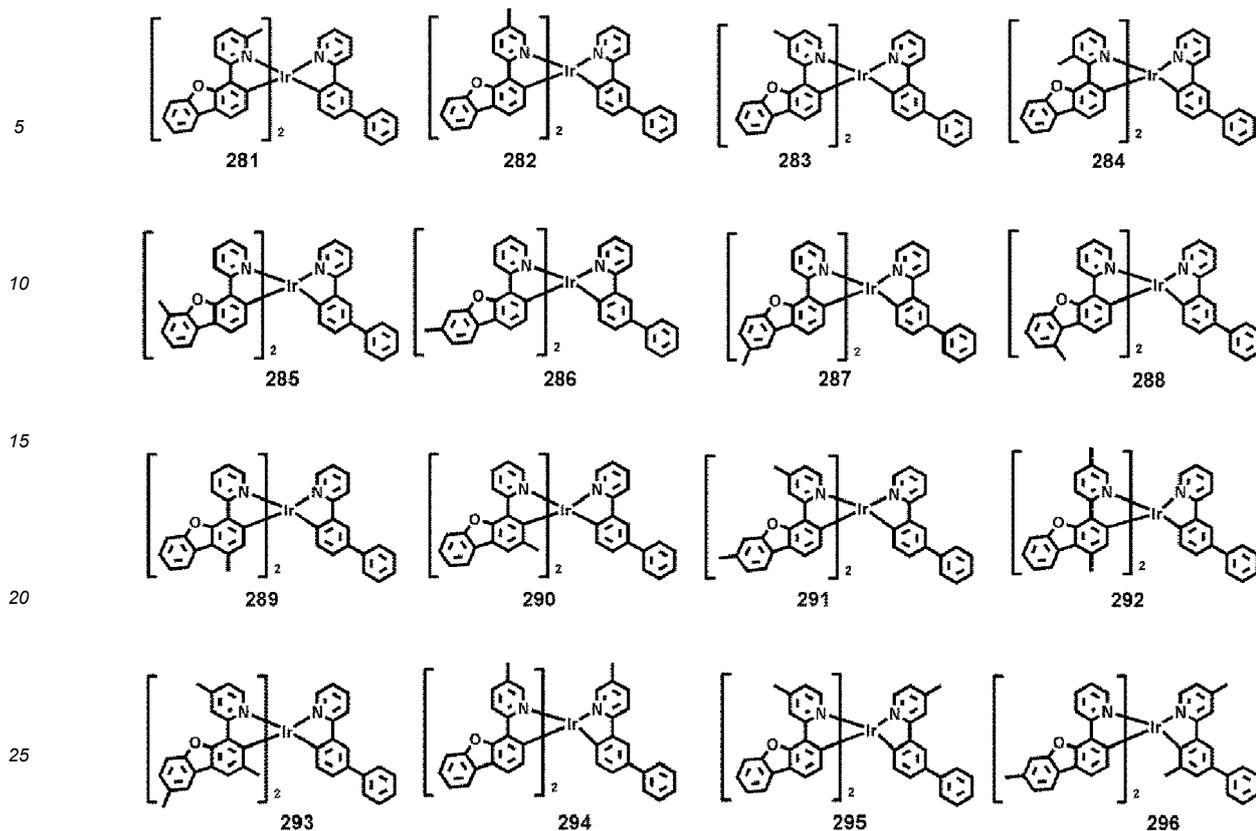


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[0073] In the organometallic compound represented by Formula 1, L_1 may be a ligand represented by Formula 2, L_2 may be a ligand represented by Formula 3, wherein R_1 , R_2 , R_{28} , R_{29} , Z_1 , and Z_2 in Formulae 2 and 3 may respectively be understood by referring to the descriptions of R_1 , R_2 , R_{28} , R_{29} , Z_1 , and Z_2 provided herein and may each not be hydrogen.

[0074] In Formula 2, the sum of a_1 and a_2 may be 1 or greater. That is, the ligand represented by Formula 2 may be substituted with at least one R_1 , R_2 , or any combination thereof (in the present specification, R_1 and R_2 may not each be hydrogen). Accordingly, an electron withdrawing group and/or an electron donating group may be introduced into the ligand represented by Formula 2. Thus, the emission wavelength of light emitted from the organometallic compound represented by Formula 1 may be precisely controlled, and electrical matching with a host may be improved. Therefore, an electronic device, e.g., an organic light-emitting device, including the organometallic compound represented by Formula 1 may emit light having excellent colorimetric purity and show effects of reducing a driving voltage.

[0075] Further, d_2 in Formula 3 may indicate the number of Z_2 (s), and d_2 may be an integer from 1 to 10. That is, since d_2 is not 0, ring CY_{12} in Formula 3 may be substituted with at least one Z_2 (in the present specification, Z_2 may not be hydrogen). Accordingly, intermolecular interaction of the organometallic compound represented by Formula 1 may be reduced and result in reduction in intermolecular stacking of the organometallic compound represented by Formula 1. Thus, the organometallic compound may emit light which may prevent spectrum broadening and have an improved full width at half maximum (FWHM). Therefore, when the organometallic compound represented by Formula 1 is used, an electronic device (e.g., an organic light-emitting device) with high quality may be manufactured.

[0076] Further, in Formulae 2 and 3, a "saturated cyclic group (e.g., a non-aromatic cyclic group)" may not be included in the list of R_1 , R_2 , R_{28} , R_{29} , Z_1 , and Z_2 . That is, the ligand included in Formula 1 may not include a "saturated cyclic group (e.g., a non-aromatic cyclic group)" as a substituent. Upon deposition of the organometallic compound represented by Formula 1, various side effects (e.g., ligand exchanging) due to an increase in deposition temperature and molecular liquefaction at a high temperature may be prevented. Thus, when the organometallic compound represented by Formula 1 is used, process stability of an organic light-emitting device may be secured.

[0077] The HOMO energy level, LUMO energy level, energy band gap, and S_1 and T_1 energy levels of some of the organometallic compounds represented by Formula 1 were evaluated by using Gaussian 09 that performs molecular structure optimizations according to density functional theory (DFT) at a degree of B3LYP. The results thereof are shown in Table 1.

Table 1

Compound No.	HOMO (eV)	LUMO (eV)	Energy band gap (eV)	S ₁ energy level (eV)	T ₁ energy level (eV)
1	-4.832	-1.231	3.601	2.831	2.504
2	-4.716	-1.165	3.551	2.835	2.485
3	-4.677	-1.111	2.566	2.868	2.508
4	-4.663	-1.118	3.545	2.807	2.477
5	-4.732	-1.168	3.564	2.844	2.484
6	-4.700	-1.158	3.542	2.818	2.475
7	-4.772	-1.248	3.524	2.826	2.489
8	-4.791	-1.256	3.536	2.837	2.496
9	-4.673	-1.196	3.477	2.812	2.532

[0078] Referring to the results of Table 1, the organometallic compound represented by Formula 1 was found to have suitable electrical characteristics for use as a dopant in an electronic device, e.g., an organic light-emitting device.

[0079] A method of synthesizing the organometallic compound represented by Formula 1 may be apparent to one of ordinary skill in the art by referring to Synthesis Examples provided herein.

[0080] The organometallic compound represented by Formula 1 may be suitable for use in an organic layer of an organic light-emitting device, for example, as a dopant in an emission layer of the organic layer. Thus, according to another aspect, there is provided an organic light-emitting device that may include a first electrode; a second electrode; and an organic layer disposed between the first electrode and the second electrode and including an emission layer, the organic layer including at least one organometallic compound represented by Formula 1.

[0081] Since the organic light-emitting device has an organic layer including the organometallic compound represented by Formula 1, the organic light-emitting device may have a low driving voltage, high external quantum efficiency, long lifespan, and low roll-off ratio.

[0082] The organometallic compound represented by Formula 1 may be used with a pair of electrodes of an organic light-emitting device. For example, the organometallic compound represented by Formula 1 may be included in the emission layer. In this embodiment, the organometallic compound may serve as a dopant and the emission layer may further include a host (that is, an amount of the organometallic compound represented by Formula 1 may be smaller than that of the host). The emission layer may emit red light or green light, e.g., red light or green light having a maximum emission wavelength of about 500 nanometers (nm) or longer, e.g., about 500 nm to about 650 nm.

[0083] As used herein, the expression the "(organic layer) includes at least one organometallic compound" may be construed as meaning the "(organic layer) may include one organometallic compound of Formula 1 or two different organometallic compounds of Formula 1".

[0084] For example, Compound 1 may only be included in the organic layer as an organometallic compound. In this embodiment, Compound 1 may be included in the emission layer of the organic light-emitting device. In some embodiments, Compounds 1 and 2 may be included in the organic layer as organometallic compounds. In this embodiment, Compounds 1 and 2 may both be included in the same layer (for example, both Compounds 1 and 2 may be included in the emission layer).

[0085] The first electrode may be an anode, which is a hole injection electrode, and the second electrode may be a cathode, which is an electron injection electrode. In some embodiments, the first electrode may be a cathode, which is an electron injection electrode, and the second electrode may be an anode, which is a hole injection electrode.

[0086] For example, in the organic light-emitting device, the first electrode may be an anode, the second electrode may be a cathode, and the organic layer may further include a hole transport region disposed between the first electrode and the emission layer and an electron transport region disposed between the emission layer and the second electrode, wherein the hole transport region may include a hole injection layer, a hole transport layer, an electron blocking layer, a buffer layer, or a combination thereof, and the electron transport region may include a hole blocking layer, an electron transport layer, an electron injection layer, or a combination thereof.

[0087] The term "organic layer" as used herein refers to a single and/or a plurality of layers between the first electrode and the second electrode in an organic light-emitting device. The "organic layer" may include not only organic compounds but also organometallic complexes including metals.

[0088] The FIGURE illustrates a schematic cross-sectional view of an organic light-emitting device 10 according to an embodiment. Hereinafter, a structure of an organic light-emitting device according to one or more embodiments and

a method of manufacturing the organic light-emitting device will be described with reference to the FIGURE. The organic light-emitting device 10 may include a first electrode 11, an organic layer 15, and a second electrode 19, which may be sequentially layered in this stated order.

5 [0089] A substrate may be additionally disposed under the first electrode 11 or on the second electrode 19. The substrate may be a conventional substrate used in organic light-emitting devices, e.g., a glass substrate or a transparent plastic substrate, each having excellent mechanical strength, thermal stability, transparency, surface smoothness, ease of handling, and water repellency.

10 [0090] The first electrode 11 may be formed by depositing or sputtering, onto the substrate, a material for forming the first electrode 11. The first electrode 11 may be an anode. The material for forming the first electrode 11 may be selected from materials with a high work function for easy hole injection. The first electrode 11 may be a reflective electrode, a semi-transmissive electrode, or a transmissive electrode. The material for forming the first electrode 11 may be selected from indium tin oxide (ITO), indium zinc oxide (IZO), tin oxide (SnO₂), and zinc oxide (ZnO). In some embodiments, the material for forming the first electrode 11 may be a metal, such as magnesium (Mg), aluminum (Al), aluminum-lithium (Al-Li), calcium (Ca), magnesium-indium (Mg-In), or magnesium-silver (Mg-Ag).

15 [0091] The first electrode 11 may have a single-layered structure or a multi-layered structure including a plurality of layers. In some embodiments, the first electrode 11 may have a triple-layered structure of ITO/Ag/ITO, but embodiments are not limited thereto.

[0092] The organic layer 15 may be on the first electrode 11.

[0093] The organic layer 15 may include a hole transport region, an emission layer, and an electron transport region.

20 [0094] The hole transport region may be between the first electrode 11 and the emission layer.

[0095] The hole transport region may include a hole injection layer, a hole transport layer, an electron blocking layer, a buffer layer, or a combination thereof.

25 [0096] The hole transport region may include a hole injection layer only or a hole transport layer only. In some embodiments, the hole transport region may include a hole injection layer and a hole transport layer which are sequentially stacked on the first electrode 11. In some embodiments, the hole transport region may include a hole injection layer, a hole transport layer, and an electron blocking layer, which are sequentially stacked on the first electrode 11.

[0097] When the hole transport region includes a hole injection layer, the hole injection layer may be formed on the first electrode 11 by using one or more suitable methods, such as vacuum deposition, spin coating, casting, and Langmuir-Blodgett (LB) deposition.

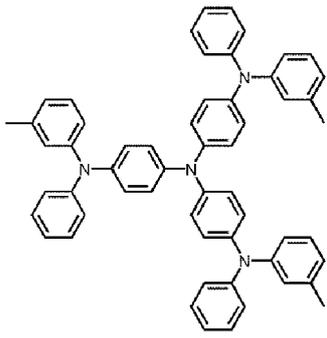
30 [0098] When a hole injection layer is formed by vacuum deposition, for example, the vacuum deposition may be performed at a deposition temperature in a range of about 100°C to about 500°C, at a vacuum pressure in a range of about 10⁻⁸ torr to about 10⁻³ torr, and at a deposition rate in a range of about 0.01 Angstroms per second (Å/sec) to about 100 Å/sec, though the conditions may vary depending on a compound that is used as a hole injection material and a structure and thermal properties of a desired hole injection layer, but conditions for the vacuum deposition are not limited thereto.

35 [0099] When a hole injection layer is formed by spin coating, the spin coating may be performed at a coating rate in a range of about 2,000 revolutions per minute (rpm) to about 5,000 rpm, and at a temperature in a range of about 80 °C to 200 °C, to facilitate removal of a solvent after the spin coating, though the conditions may vary depending on a compound that is used as a hole injection material and a structure and thermal properties of a desired hole injection layer, but conditions for the spin coating are not limited thereto.

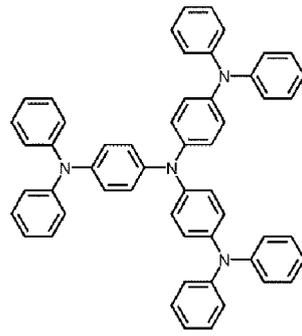
40 [0100] The conditions for forming a hole transport layer and an electron blocking layer may be inferred from the conditions for forming the hole injection layer.

45 [0101] The hole transport region may include m-MTDATA, TDATA, 2-TNATA, NPB, β-NPB, TPD, spiro-TPD, spiro-NPB, methylated-NPB, TAPC, HMTPD, 4,4',4''-tris(N-carbazolyl)triphenylamine (TCTA), polyaniline/dodecylbenzenesulfonic acid (PANI/DBSA), poly(3,4-ethylenedioxythiophene)/poly(4-styrenesulfonate) (PEDOT/PSS), polyaniline/camphor-sulfonic acid (PANI/CSA), polyaniline/poly(4-styrene sulfonate) (PANI/PSS), a compound represented by Formula 201, a compound represented by Formula 202, or any combination thereof.

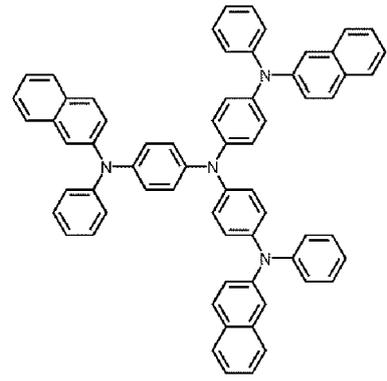
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m-MTDATA



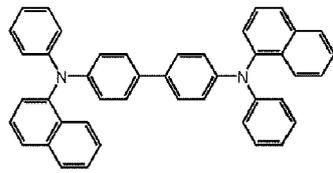
TDATA



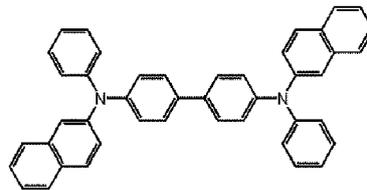
2-TNATA

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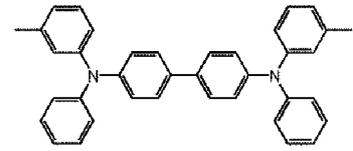
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NPB



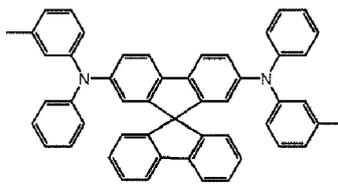
β -NPB



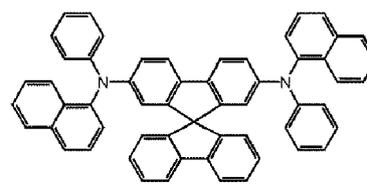
TPD

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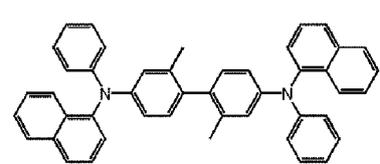
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Spiro-TPD



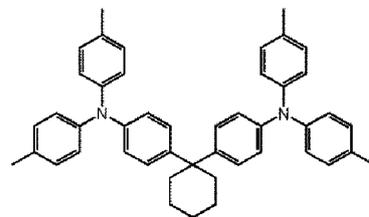
Spiro-NPB



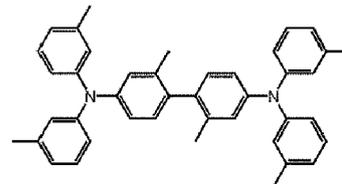
methylated NPB

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TAPC



HMTPD

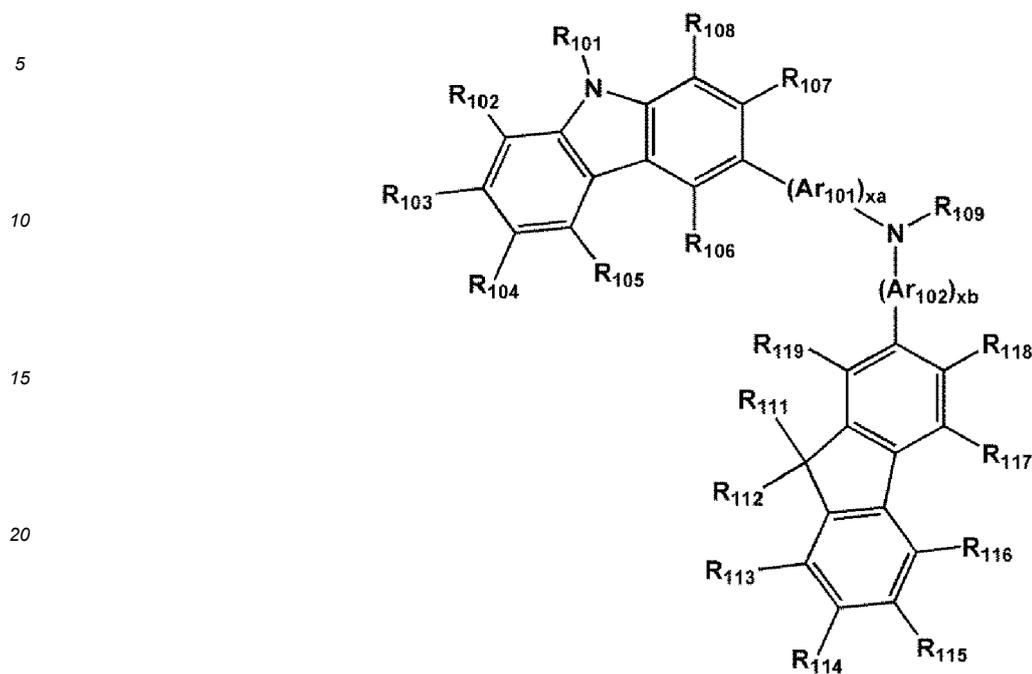
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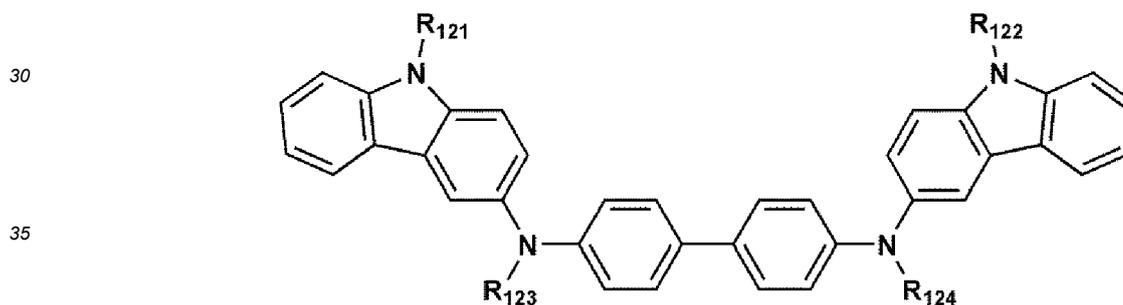
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Formula 201



Formula 202



40 **[0102]** In Formula 201, Ar₁₀₁ and Ar₁₀₂ may each independently be a phenylene group, a pentalenylene group, an indenylene group, a naphthylene group, an azulenylene group, a heptalenylene group, an acenaphthylene group, a fluorenylene group, a phenalenylene group, a phenanthrenylene group, an anthracenylene group, a fluoranthenylene group, a triphenylenylene group, a pyrenylene group, a chrysenylenylene group, a naphthacenylene group, a picenylene group, a perylenylene group, or a pentacenylene group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, a C₁-C₆₀ alkoxy group, a C₃-C₁₀ cycloalkyl group, a C₃-C₁₀ cycloalkenyl group, a C₁-C₁₀ heterocycloalkyl group, a C₂-C₁₀ heterocycloalkenyl group, a C₆-C₆₀ aryl group, a C₆-C₆₀ aryloxy group, a C₆-C₆₀ arylthio group, a C₁-C₆₀ heteroaryl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, or any combination thereof.

50 **[0103]** In Formula 201, xa and xb may each independently be an integer from 0 to 5. In some embodiments, xa and xb may each independently be an integer from 0 to 2. In some embodiments, xa may be 1, and xb may be 0, but embodiments are not limited thereto.

[0104] In Formulae 201 and 202, R₁₀₁ to R₁₀₈, R₁₁₁ to R₁₁₉, and R₁₂₁ to R₁₂₄ may each independently be:

55 hydrogen, deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₁₀ alkyl group (e.g., a methyl group, an ethyl group, a propyl group, a butyl group, pentyl group, or a hexyl group), or a C₁-C₁₀ alkoxy group (e.g., a methoxy group, an

ethoxy group, a propoxy group, a butoxy group, or a pentoxy group);

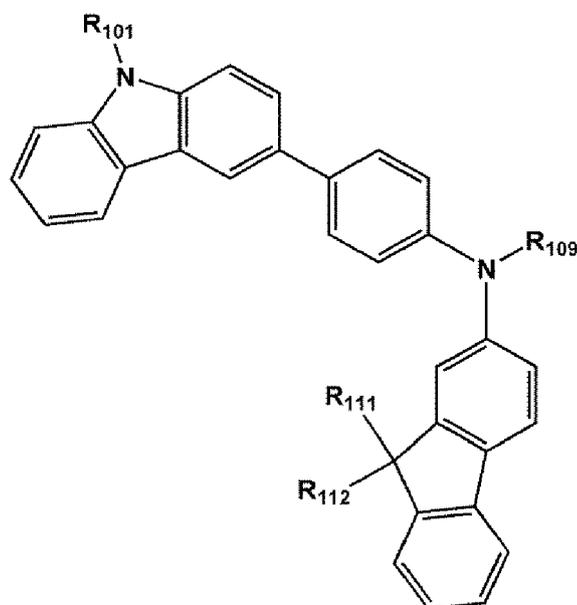
a C₁-C₁₀ alkyl group or a C₁-C₁₀ alkoxy group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, or any combination thereof; or

a phenyl group, a naphthyl group, an anthracenyl group, a fluorenyl group, or a pyrenyl group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₁₀ alkyl group, a C₁-C₁₀ alkoxy group, or any combination thereof.

[0105] In Formula 201, R₁₀₉ may be a phenyl group, a naphthyl group, an anthracenyl group, or a pyridinyl group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₂₀ alkyl group, a C₁-C₂₀ alkoxy group, a phenyl group, a naphthyl group, an anthracenyl group, a pyridinyl group, or any combination thereof.

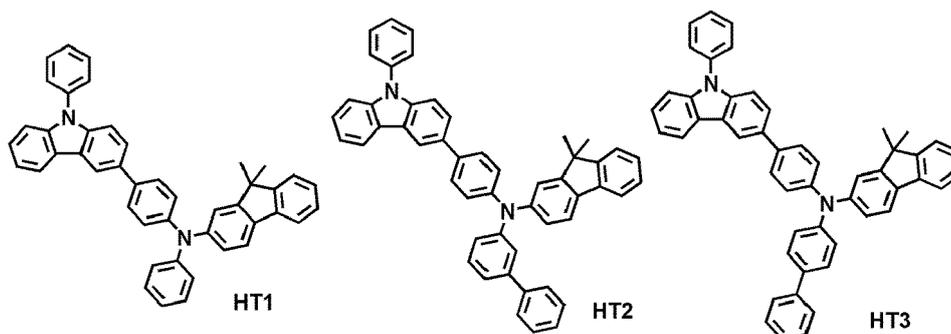
[0106] In some embodiments, the compound represented by Formula 201 may be represented by Formula 201A:

Formula 201A

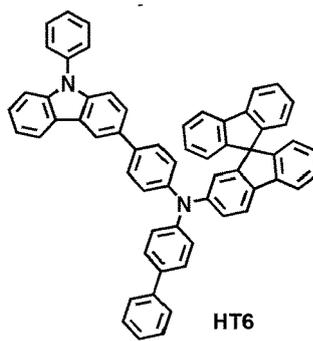
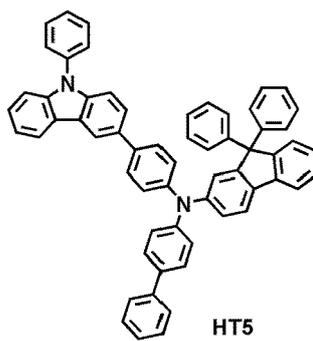
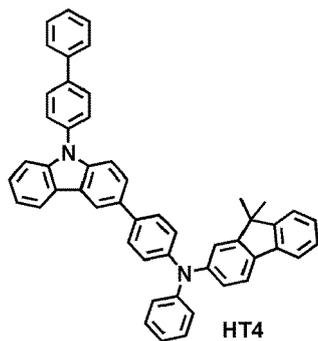


[0107] In Formula 201A, R₁₀₁, R₁₁₁, R₁₁₂, and R₁₀₉ may respectively be understood by referring to the descriptions of R₁₀₁, R₁₁₁, R₁₁₂, and R₁₀₉ provided herein.

[0108] In some embodiments, the hole transport region may include one of Compounds HT1 to HT20 or any combination thereof:

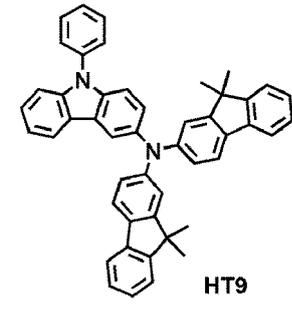
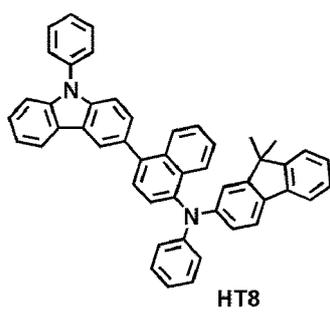
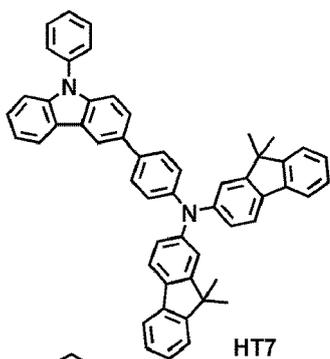


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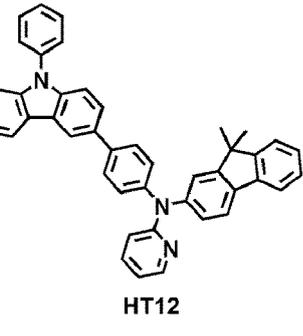
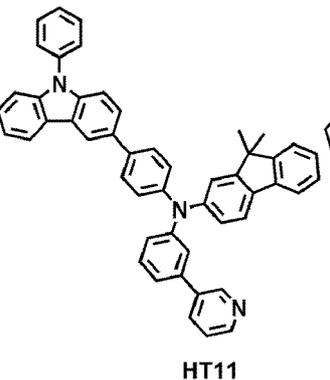
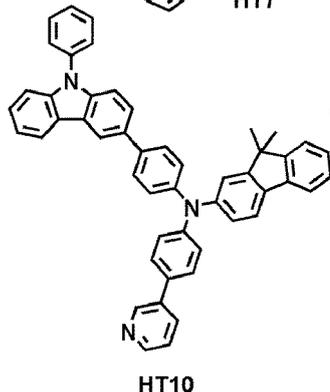
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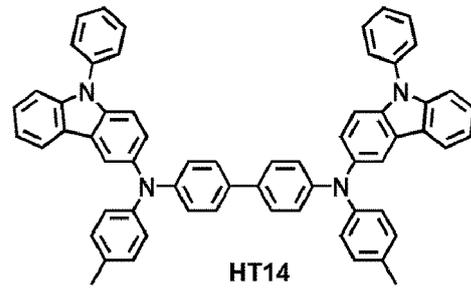
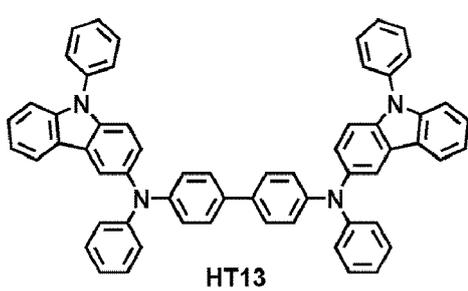
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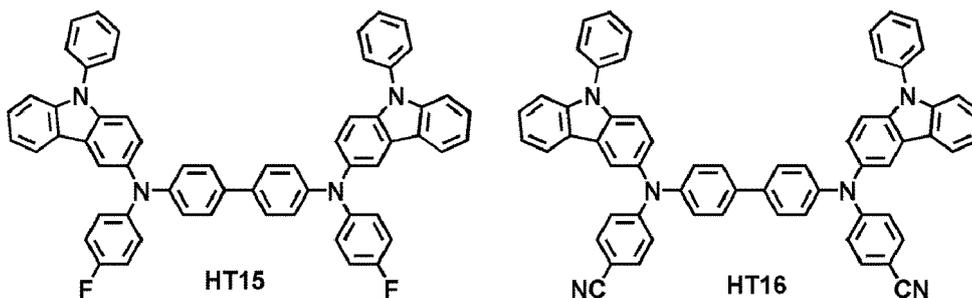
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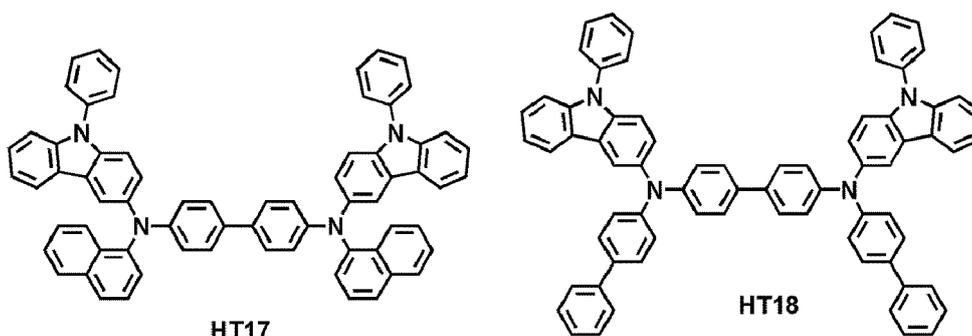
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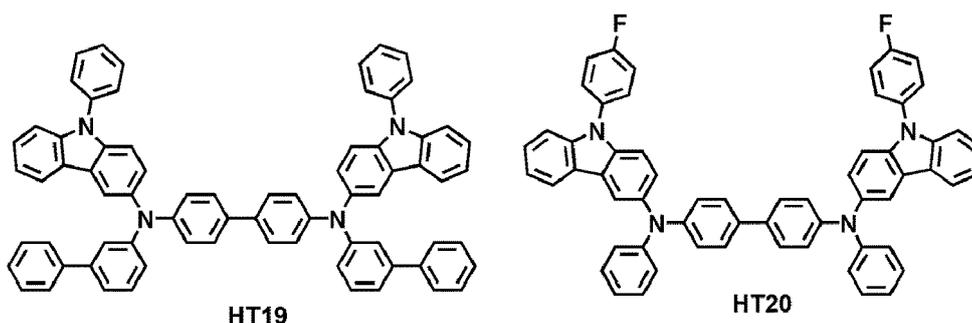
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[0109] The thickness of the hole transport region may be in a range of about 100 (Angstroms) Å to about 10,000 Å, and in some embodiments, about 100 Å to about 1,000 Å. When the hole transport region includes at least one selected from a hole injection layer and a hole transport layer, the thickness of the hole injection layer may be in a range of about 100 Å to about 10,000 Å, and in some embodiments, about 100 Å to about 1,000 Å, and the thickness of the hole transport layer may be in a range of about 50 Å to about 2,000 Å, and in some embodiments, about 100 Å to about 1,500 Å. When the thicknesses of the hole transport region, the hole injection layer, and the hole transport layer are within any of these ranges, excellent hole transport characteristics may be obtained without a substantial increase in driving voltage.

40

[0110] The hole transport region may include a charge generating material as well as the aforementioned materials, to improve conductive properties of the hole transport region. The charge generating material may be substantially homogeneously or non-homogeneously dispersed in the hole transport region.

45

[0111] The charge generating material may include, for example, a p-dopant. The p-dopant may be a quinone derivative, a metal oxide, a compound containing a cyano group, or any combination thereof, but embodiments are not limited thereto. In some embodiments, the p-dopant may be a quinone derivative, such as tetracyanoquinodimethane (TCNQ), a 2,3,5,6-tetrafluoro-tetracyano-1,4-benzoquinodimethane (F4-TCNQ), or F6-TCNQ; a metal oxide, such as a tungsten oxide or a molybdenum oxide; a compound containing a cyano group, such as Compound HT-D1; or any combination thereof.

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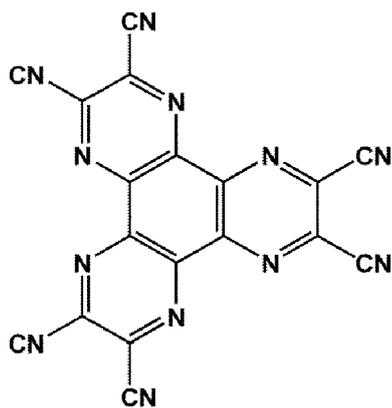
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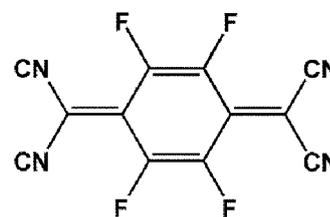
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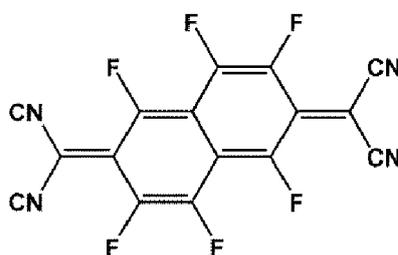
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HT-D1



F4-TCNQ



F6-TCNNQ

[0112] The hole transport region may further include a buffer layer.

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[0113] The buffer layer may compensate for an optical resonance distance depending on a wavelength of light emitted from the emission layer to improve the efficiency of an organic light-emitting device.

[0114] When the hole transport region includes an electron blocking layer, a material for forming the electron blocking layer may be selected from the materials for forming a hole transport region and host materials described herein, but embodiments are not limited thereto. In some embodiments, when the hole transport region includes an electron blocking layer, mCP described herein may be used for forming the electron blocking layer.

35

[0115] An emission layer may be formed on the hole transport region by using one or more suitable methods, such as vacuum deposition, spin coating, casting, or LB deposition. When the emission layer is formed by vacuum deposition or spin coating, vacuum deposition and coating conditions for forming the emission layer may be generally similar to those conditions for forming a hole injection layer, though the conditions may vary depending on a compound that is used.

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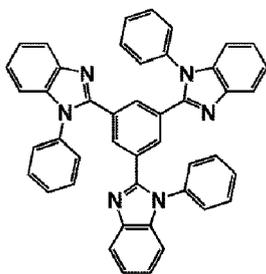
[0116] The emission layer may include a host and a dopant, and the dopant may include the organometallic compound represented by Formula 1.

[0117] The host may include TPBi, TBADN, ADN (also known as "DNA"), CBP, CDBP, TCP, mCP, Compound H50, Compound H51, Compound H52, or any combination thereof:

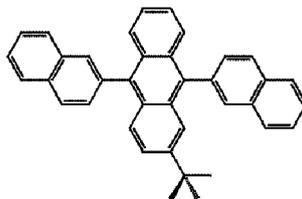
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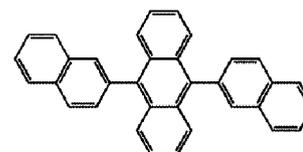
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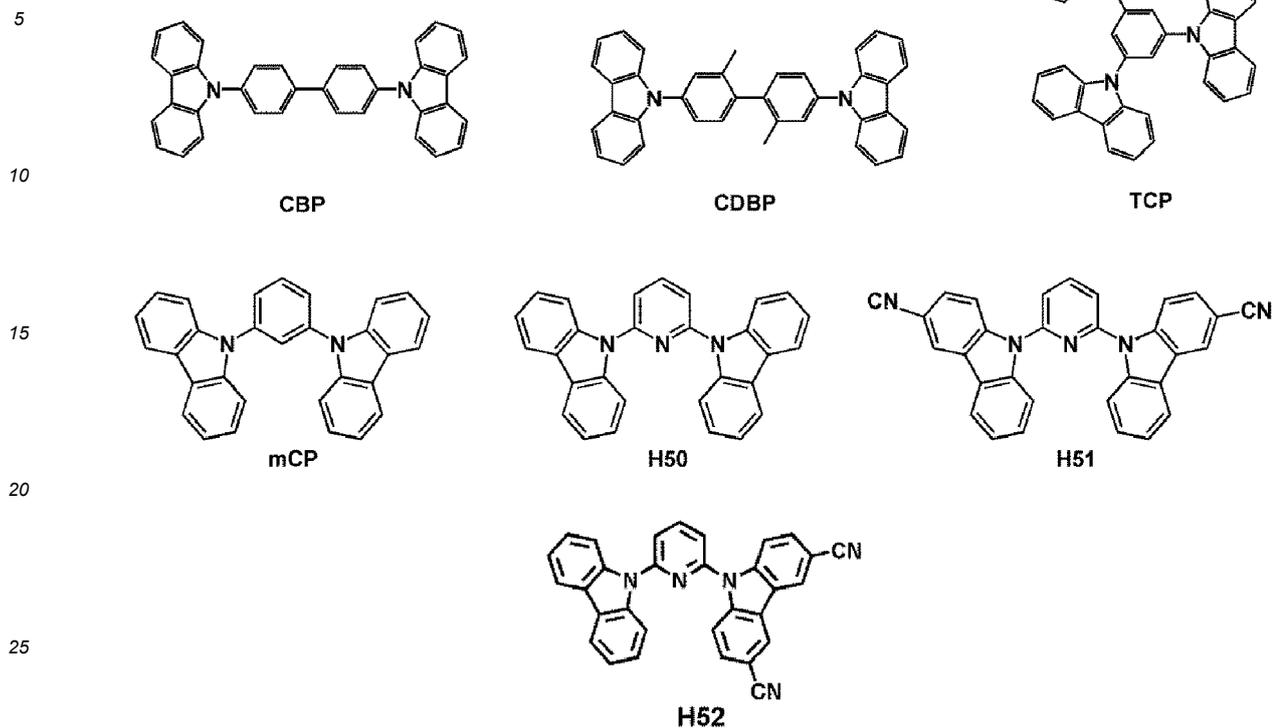
TPBi



TBADN



ADN



[0118] When the organic light-emitting device 10 is a full-color organic light-emitting device, the emission layer may be patterned into a red emission layer, a green emission layer, and/or a blue emission layer. In some embodiments, the emission layer may have a structure in which the red emission layer, the green emission layer, and/or the blue emission layer are layered to emit white light. In some embodiments, the structure of the emission layer may vary.

[0119] When the emission layer includes the host and the dopant, an amount of the dopant may be from about 0.01 parts to about 15 parts by weight based on about 100 parts by weight of the host, but embodiments are not limited thereto.

[0120] The thickness of the emission layer may be in a range of about 100 Å to about 1,000 Å, and in some embodiments, about 200 Å to about 600 Å. When the thickness of the emission layer is within any of these ranges, improved luminescence characteristics may be obtained without a substantial increase in driving voltage.

[0121] Next, an electron transport region may be formed on the emission layer.

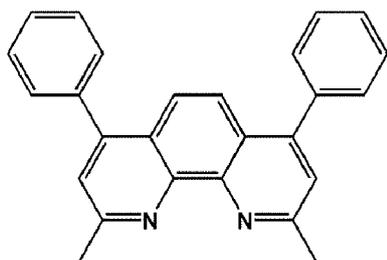
[0122] The electron transport region may include a hole blocking layer, an electron transport layer, an electron injection layer, or a combination thereof.

[0123] In some embodiments, the electron transport region may have a hole blocking layer/an electron transport layer/an electron injection layer structure or an electron transport layer/an electron injection layer structure, but embodiments are not limited thereto. The electron transport layer may have a single-layered structure or a multi-layered structure including two or more different materials.

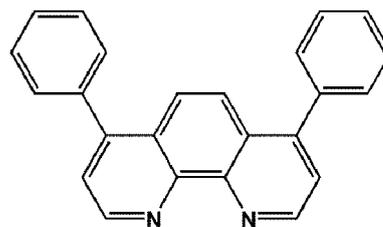
[0124] The conditions for forming a hole blocking layer, an electron transport layer, and an electron injection layer may be inferred based on the conditions for forming the hole injection layer.

[0125] When the electron transport region includes a hole blocking layer, the hole blocking layer may include, for example, at least of BCP, Bphen, BAiq, or any combination thereof:

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BCP



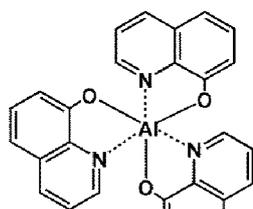
Bphen

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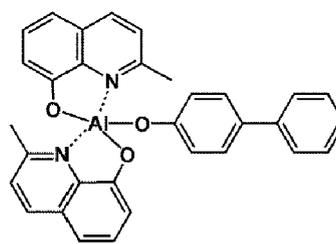
[0126] The thickness of the hole blocking layer may be in a range of about 20 Å to about 1,000 Å, and in some embodiments, about 30 Å to about 300 Å. When the thickness of the hole blocking layer is within any of these ranges, excellent hole blocking characteristics may be obtained without a substantial increase in driving voltage.

[0127] The electron transport layer may include BCP, Bphen, TPBi, Alq₃, BAq, TAZ, NTAZ, or any combination thereof:

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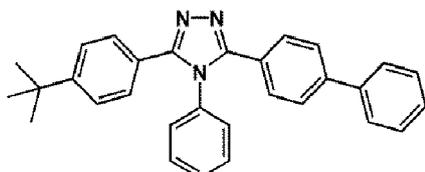
Alq₃



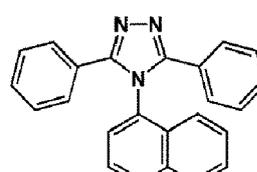
BAq

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TAZ

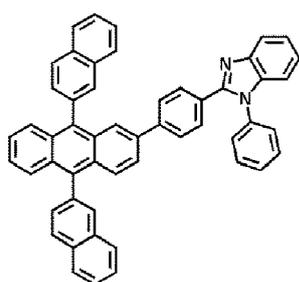


NTAZ

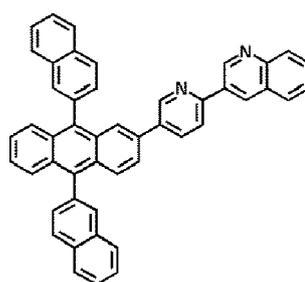
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[0128] In some embodiments, the electron transport layer may include at least one of Compounds ET1 to ET25, but embodiments are not limited thereto:

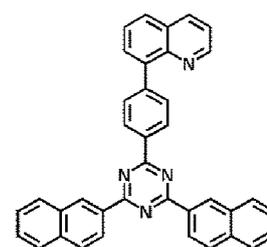
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ET1



ET2



ET3

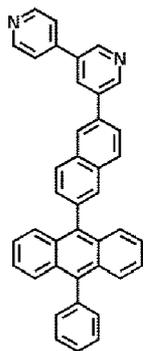
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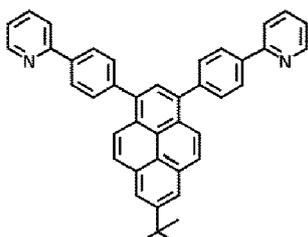
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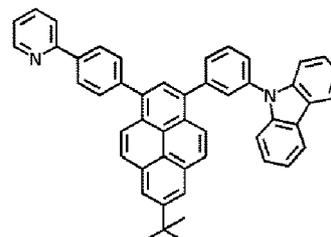
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ET4

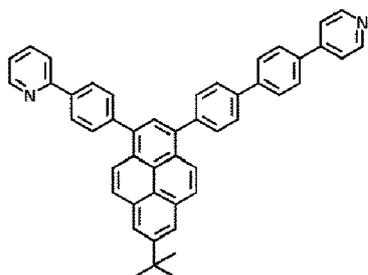


ET5

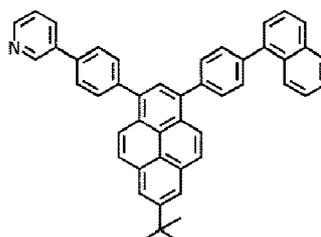


ET6

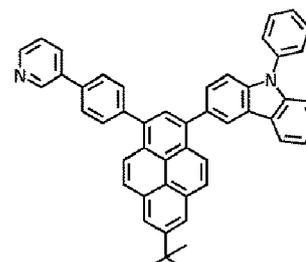
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ET7

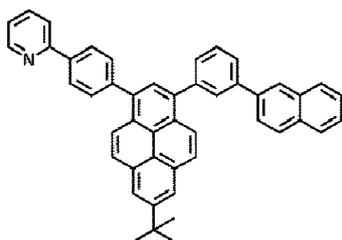


ET8

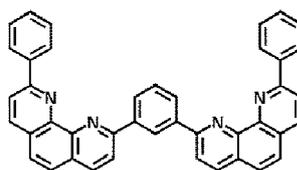


ET9

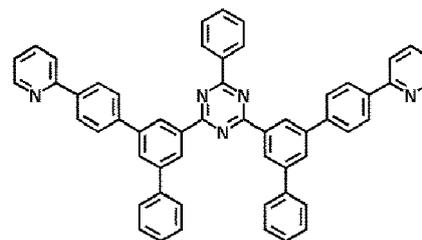
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ET10

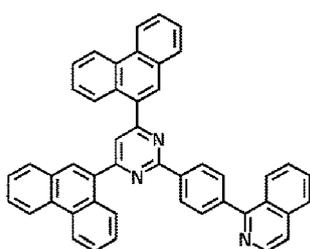


ET11

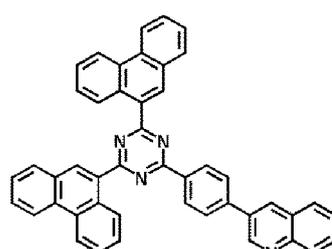


ET12

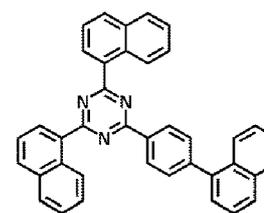
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ET13



ET14



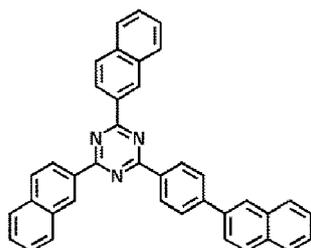
ET15

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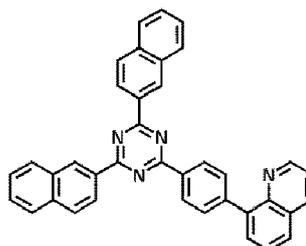
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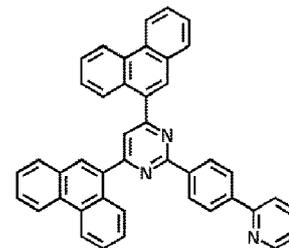
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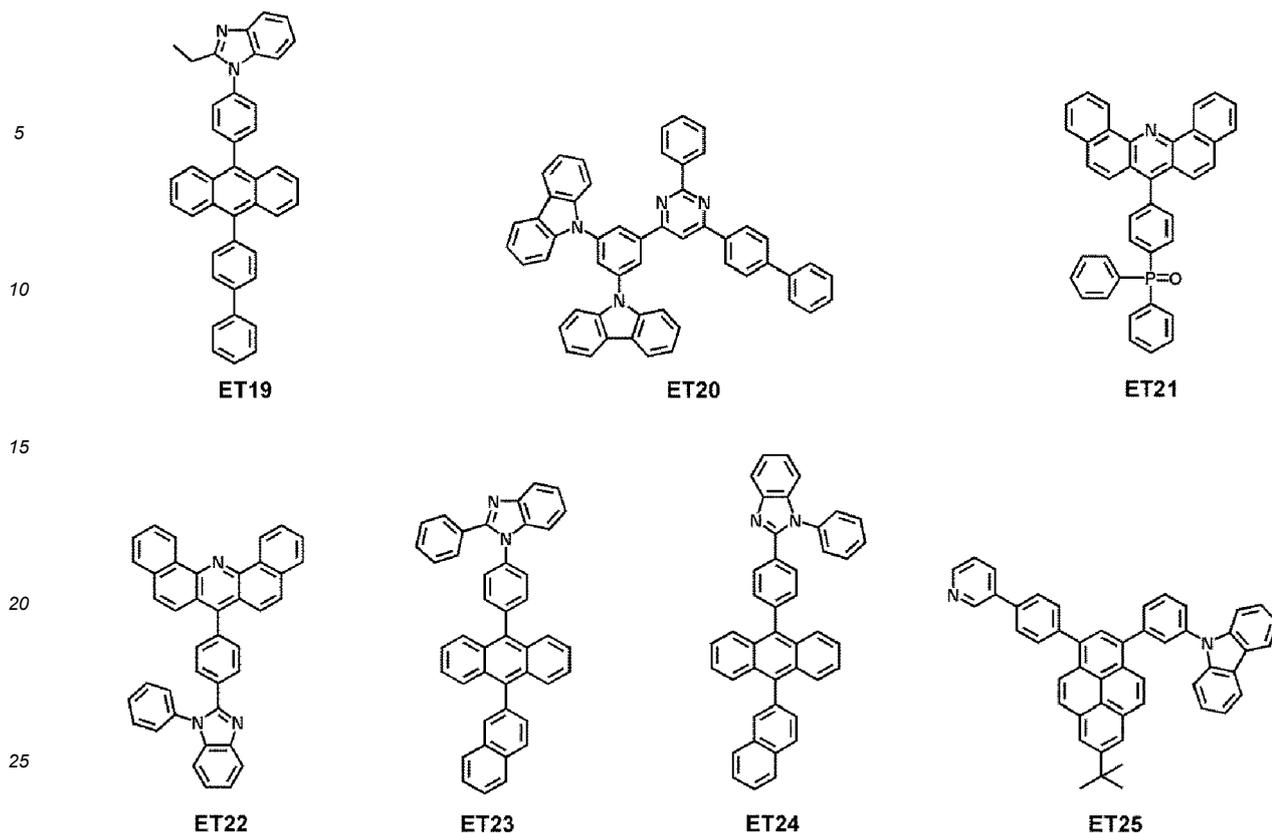
ET16



ET17



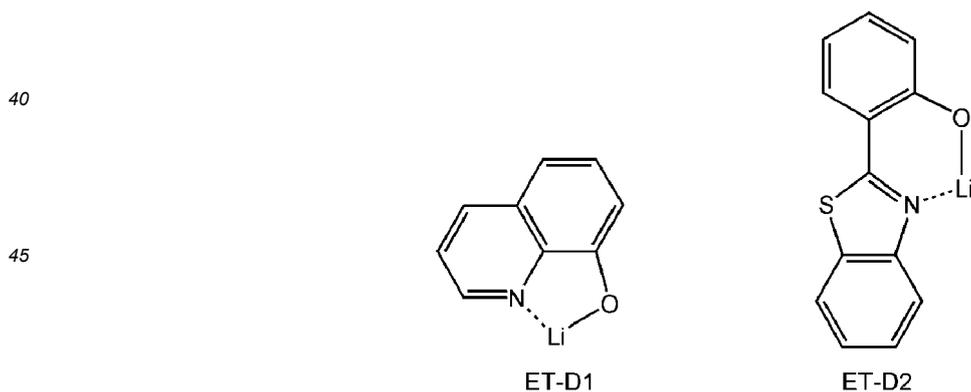
ET18



[0129] The thickness of the electron transport layer may be in a range of about 100 Å to about 1,000 Å, and in some embodiments, about 150 Å to about 500 Å. When the thickness of the electron transport layer is within any of these ranges, excellent electron transport characteristics may be obtained without a substantial increase in driving voltage.

[0130] The electron transport layer may further include a material containing metal, in addition to the materials described above.

[0131] The material containing metal may include a Li complex. The Li complex may include, e.g., Compound ET-D1 or Compound ET-D2:



[0132] The electron transport region may include an electron injection layer that facilitates electron injection from the second electrode 19.

[0133] The electron injection layer may include LiF, NaCl, CsF, Li₂O, BaO, or any combination thereof.

[0134] The thickness of the electron injection layer may be in a range of about 1 Å to about 100 Å, for example, about 3 Å to about 90 Å. When the thickness of the electron injection layer is within any of these ranges, excellent electron injection characteristics may be obtained without a substantial increase in driving voltage.

[0135] The second electrode 19 may be on the organic layer 15. The second electrode 19 may be a cathode. A material for forming the second electrode 19 may be a material with a relatively low work function, such as a metal, an alloy, an

electrically conductive compound, and a mixture thereof. Examples of the material for forming the second electrode 19 may include lithium (Li), magnesium (Mg), aluminum (Al), aluminum-lithium (Al-Li), calcium (Ca), magnesium-indium (Mg-In), and magnesium-silver (Mg-Ag). In some embodiments, ITO or IZO may be used to form a transmissive second electrode 19 to manufacture a top emission light-emitting device. In some embodiments, the material for forming the

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second electrode 19 may vary.

[0136] Hereinbefore the organic light-emitting device 10 has been described with reference to the FIGURE, but embodiments are not limited thereto.

[0137] According to an aspect of still another embodiment, a diagnostic composition may include at least one organometallic compound represented by Formula 1.

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[0138] Since the organometallic compound represented by Formula 1 provides high luminescence efficiency, the diagnostic efficiency of the diagnostic composition that includes the organometallic compound represented by Formula 1 may be excellent.

[0139] The diagnostic composition may be applied in various ways, such as in a diagnostic kit, a diagnostic reagent, a biosensor, or a biomarker.

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[0140] The term "C₁-C₆₀ alkyl group" as used herein refers to a linear or branched saturated aliphatic hydrocarbon monovalent group having 1 to 60 carbon atoms. The term "C₁-C₆₀ alkylene group" as used herein refers to a divalent group having the same structure as the C₁-C₆₀ alkyl group.

[0141] Examples of the C₁-C₆₀ alkyl group, the C₁-C₂₀ alkyl group, and/or the C₁-C₁₀ alkyl group as used herein may include a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an isobutyl group, a tert-butyl group, an n-pentyl group, a tert-pentyl group, a neopentyl group, an isopentyl group, a sec-pentyl group, a 3-pentyl group, a sec-isopentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group, a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group, a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decyl group, an iso-decyl group, a sec-decyl group or a tert-decyl group, each unsubstituted or substituted

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with a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an isobutyl group, a tert-butyl group, an n-pentyl group, a tert-pentyl group, a neopentyl group, an isopentyl group, a sec-pentyl group, a 3-pentyl group, a sec-isopentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group, a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group, a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decyl group, an iso-decyl group, a sec-decyl group, a tert-decyl group, or any combination thereof. In some

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embodiments, Formula 9-33 described above may be a branched C₆ alkyl group. Formula 9-33 may be a tert-butyl group substituted with two methyl groups.

[0142] The term "C₁-C₆₀ alkoxy group" as used herein refers to a monovalent group represented by -OA₁₀₁ (wherein A₁₀₁ is a C₁-C₁ alkyl group).

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[0143] Examples of the C₁-C₆₀ alkoxy group, the C₁-C₂₀ alkoxy group, or the C₁-C₁₀ alkoxy group as used herein may include a methoxy group, an ethoxy group, a propoxy group, a butoxy group, or a pentoxy group.

[0144] The term "C₂-C₆₀ alkenyl group" as used herein refers to a group formed by placing at least one carbon-carbon double bond in the middle or at the terminus of the C₂-C₆₀ alkyl group. Examples thereof include an ethenyl group, a propenyl group, and a butenyl group. The term "C₂-C₆₀ alkenylene group" as used herein refers to a divalent group

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having the same structure as the C₂-C₆₀ alkenyl group.

[0145] The term "C₂-C₆₀ alkynyl group" as used herein refers to a group formed by placing at least one carbon-carbon triple bond in the middle or at the terminus of the C₂-C₆₀ alkyl group. Examples thereof include an ethenyl group and a propenyl group. The term "C₂-C₆₀ alkynylene group" as used herein refers to a divalent group having the same structure as the C₂-C₆₀ alkynyl group.

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[0146] The term "C₃-C₁₀ cycloalkyl group" as used herein refers to a monovalent monocyclic saturated hydrocarbon group including 3 to 10 carbon atoms. The term "C₃-C₁₀ cycloalkylene group" as used herein refers to a divalent group having the same structure as the C₃-C₁₀ cycloalkyl group.

[0147] Examples of the C₃-C₁₀ cycloalkyl group as used herein may include a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a bicyclo[1.1.1]pentyl group, a bicyclo[2.1.1]hexyl group, a bicyclo[2.2.1]heptyl group (a norbornanyl group), or a bicyclo[2.2.2]octyl group.

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[0148] The term "C₁-C₁₀ heterocycloalkyl group" as used herein refers to a monovalent monocyclic group including at least one N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof as a ring-forming atom and 1 to 10 carbon atoms. The term "C₁-C₁₀ heterocycloalkylene group" as used herein refers to a divalent group having the same structure as the C₁-C₁₀ heterocycloalkyl group.

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[0149] Examples of the C₁-C₁₀ heterocycloalkyl group as used herein may include a silolanyl group, a silinanyl group, a tetrahydrofuranyl group, a tetrahydro-2H-pyrananyl group, or a tetrahydrothiophenyl group.

[0150] The term "C₃-C₁₀ cycloalkenyl group" as used herein refers to a monovalent monocyclic group that has 3 to

10 carbon atoms and at least one carbon-carbon double bond in its ring, wherein the molecular structure as a whole is non-aromatic. Examples thereof include a cyclopentenyl group, a cyclohexenyl group, and a cycloheptenyl group. The term "C₃-C₁₀ cycloalkenylene group" as used herein refers to a divalent group having the same structure as the C₃-C₁₀ cycloalkenyl group.

5 **[0151]** The term "C₂-C₁₀ heterocycloalkenyl group" as used herein refers to a monovalent monocyclic group including at least one N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof as a ring-forming atom, 2 to 10 carbon atoms, and at least one double bond in its ring. Examples of the C₂-C₁₀ heterocycloalkenyl group include a 2,3-dihydrofuranyl group and a 2,3-dihydrothiophenyl group. The term "C₁-C₁₀ heterocycloalkylene group" as used herein refers to a divalent group having the same structure as the C₁-C₁₀ heterocycloalkyl group.

10 **[0152]** The term "C₆-C₆₀ aryl group" as used herein refers to a monovalent group having a carbocyclic aromatic system having 6 to 60 carbon atoms. The term "C₆-C₆₀ arylene group" as used herein refers to a divalent group having a carbocyclic aromatic system having 6 to 60 carbon atoms. Examples of the C₆-C₆₀ aryl group include a phenyl group, a naphthyl group, an anthracenyl group, a phenanthrenyl group, a pyrenyl group, and a chrysenyl group. When the C₆-C₆₀ aryl group and the C₆-C₆₀ arylene group each include a plurality of rings, the plurality of rings may be fused to each other.

15 **[0153]** The term "C₇-C₆₀ alkyl aryl group" as used herein refers to a C₆-C₆₀ aryl group substituted with at least one C₁-C₆₀ alkyl group.

20 **[0154]** The term "C₁-C₆₀ heteroaryl group" as used herein refers to a monovalent group having a heterocyclic aromatic system having at least one N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof as a ring-forming atom and 1 to 60 carbon atoms. The term "C₁-C₆₀ heteroarylene group" as used herein refers to a divalent group having a heterocyclic aromatic system having at least one heteroatom selected from N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof as a ring-forming atom and 1 to 60 carbon atoms. Examples of the C₁-C₆₀ heteroaryl group include a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, and an isoquinolinyl group. When the C₁-C₆₀ heteroaryl group and the C₁-C₆₀ heteroarylene group each include a plurality of rings, the plurality of rings may be fused to each other.

25 **[0155]** The term "C₂-C₆₀ alkyl heteroaryl group" as used herein refers to a C₁-C₆₀ heteroaryl group substituted with at least one C₁-C₆₀ alkyl group.

30 **[0156]** The term "C₆-C₆₀ aryloxy group" as used herein is represented by -OA₁₀₂ (wherein A₁₀₂ is the C₆-C₆₀ aryl group). The term "C₆-C₆₀ arylthio group" as used herein is represented by -SA₁₀₃ (wherein A₁₀₃ is the C₆-C₆₀ aryl group). The term "C₁-C₆₀ alkylthio group" as used herein is represented by -SA₁₀₄ (wherein A₁₀₄ is the C₁-C₆₀ alkyl group).

35 **[0157]** The term "monovalent non-aromatic condensed polycyclic group" as used herein refers to a monovalent group that has two or more condensed rings and only carbon atoms (e.g., the number of carbon atoms may be in a range of 8 to 60) as ring-forming atoms, wherein the molecular structure as a whole is non-aromatic. Examples of the monovalent non-aromatic condensed polycyclic group include a fluorenyl group. The term "divalent non-aromatic condensed polycyclic group" as used herein refers to a divalent group having substantially the same structure as the monovalent non-aromatic condensed polycyclic group.

40 **[0158]** The term "monovalent non-aromatic condensed heteropolycyclic group" as used herein refers to a monovalent group that has two or more condensed rings and a heteroatom of N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof and carbon atoms (e.g., the number of carbon atoms may be in a range of 1 to 60) as ring-forming atoms, wherein the molecular structure as a whole is non-aromatic. Examples of the monovalent non-aromatic condensed heteropolycyclic group include a carbazolyl group. The term "divalent non-aromatic condensed heteropolycyclic group" as used herein refers to a divalent group having substantially the same structure as the monovalent non-aromatic condensed heteropolycyclic group.

45 **[0159]** The term "C₅-C₃₀ carbocyclic group" as used herein refers to a saturated or unsaturated cyclic group including 5 to 30 carbon atoms only as ring-forming atoms. The C₅-C₃₀ carbocyclic group may be a monocyclic group or a polycyclic group. Examples of the "C₅-C₃₀ carbocyclic group (unsubstituted or substituted with at least one R_{10a})" may include an adamantane group, a norbornene group, a bicyclo[1.1.1]pentane group, a bicyclo[2.1.1]hexane group, a bicyclo[2.2.1]heptane group (a norbornane group), a bicyclo[2.2.2]octane group, a cyclopentane group, a cyclohexane group, a cyclohexene group, a benzene group, a naphthalene group, an anthracene group, a phenanthrene group, a triphenylene group, a pyrene group, a chrysene group, a 1,2,3,4-tetrahydronaphthalene group, a cyclopentadiene group, a silole group, or a fluorene group, each (unsubstituted or substituted with at least one R_{10a}).

50 **[0160]** The term "C₁-C₃₀ heterocyclic group" as used herein refers to saturated or unsaturated cyclic group including 1 to 30 carbon atoms and at least one N, O, P, Si, B, Se, Ge, Te, S, or any combination thereof as ring-forming atoms. The C₁-C₃₀ heterocyclic group may be a monocyclic group or a polycyclic group. The C₁-C₃₀ heterocyclic group may be a monocyclic group or a polycyclic group. Examples of the "C₁-C₃₀ heterocyclic group (unsubstituted or substituted with at least one R_{10a})" may include a thiophene group, a furan group, a pyrrole group, a silole group, a borole group, a phosphole group, a selenophene group, a germole group, a benzothiophene group, a benzofuran group, an indole group, an indene group, a benzosilole group, a benzoborole group, a benzophosphole group, a benzoselenophene

group, a benzogermole group, a dibenzothiophene group, a dibenzofuran group, a carbazole group, a dibenzosilole group, a dibenzoborole group, a dibenzophosphole group, a dibenzoselenophene group, a dibenzogermole group, a dibenzothiophene 5-oxide group, a 9H-fluorene-9-one group, a dibenzothiophene 5,5-dioxide group, an azabenzothiophene group, an azabenzofuran group, an azaindole group, an azaindene group, an azabenzosilole group, an azabenzoborole group, an azabenzophosphole group, an azabenzoselenophene group, an azabenzogermole group, an azadibenzothiophene group, an azadibenzofuran group, an azacarbazole group, an azafluorene group, an azadibenzosilole group, an azadibenzoborole group, an azadibenzophosphole group, an azadibenzoselenophene group, an azadibenzogermole group, an azadibenzothiophene 5-oxide group, an aza-9H-fluorene-9-one group, an azadibenzothiophene 5,5-dioxide group, a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a pyrazole group, an imidazole group, a triazole group, an oxazole group, an isooxazole group, a thiazole group, an isothiazole group, an oxadiazole group, a thiadiazole group, a benzopyrazole group, a benzimidazole group, a benzoxazole group, a benzothiazole group, a benzoxadiazole group, a benzothiadiazole group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group, each (unsubstituted or substituted with at least one R_{10a}).

[0161] The "fluorinated C₁-C₆₀ alkyl group (or fluorinated C₁-C₂₀ alkyl group or the like)", "fluorinated C₃-C₁₀ cycloalkyl group", "fluorinated C₁-C₁₀ heterocycloalkyl group", and "fluorinated phenyl group" as used herein may respectively be a C₁-C₆₀ alkyl group (or C₁-C₂₀ alkyl group or the like), C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, and a phenyl group, each substituted with at least one fluoro group (-F). Examples of the "fluorinated C₁ alkyl group (i.e., a fluorinated methyl group)" may include -CF₃, -CF₂H, and -CFH₂. The "fluorinated C₁-C₆₀ alkyl group (or fluorinated C₁-C₂₀ alkyl group or the like)", "fluorinated C₃-C₁₀ cycloalkyl group", "fluorinated C₁-C₁₀ heterocycloalkyl group", or "fluorinated phenyl group" may respectively be: i) a fully fluorinated C₁-C₆₀ alkyl group (or fully fluorinated C₁-C₂₀ alkyl group or the like), fully fluorinated C₃-C₁₀ cycloalkyl group, fully fluorinated C₁-C₁₀ heterocycloalkyl group, or fully fluorinated phenyl group, in which all hydrogen atoms are substituted with fluoro groups; or ii) a partially fluorinated C₁-C₆₀ alkyl group (or partially fluorinated C₁-C₂₀ alkyl group or the like), partially fluorinated C₃-C₁₀ cycloalkyl group, partially fluorinated C₁-C₁₀ heterocycloalkyl group, or partially fluorinated phenyl group, in which some of hydrogen atoms are substituted with fluoro groups.

[0162] The "deuterated C₁-C₆₀ alkyl group (or deuterated C₁-C₂₀ alkyl group or the like)", "deuterated C₃-C₁₀ cycloalkyl group", "deuterated C₁-C₁₀ heterocycloalkyl group", and "deuterated phenyl group" as used herein may respectively be a C₁-C₆₀ alkyl group (or C₁-C₂₀ alkyl group or the like), C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, and a phenyl group, each substituted with at least one deuterium. Examples of the "deuterated C₁ alkyl group (i.e., a deuterated methyl group)" may include -CD₃, -CD₂H, and -CDH₂. Examples of the "deuterated C₃-C₁₀ cycloalkyl group" may include Formula 10-501. The "deuterated C₁-C₆₀ alkyl group (or deuterated C₁-C₂₀ alkyl group or the like)", "deuterated C₃-C₁₀ cycloalkyl group", "deuterated C₁-C₁₀ heterocycloalkyl group", or "deuterated phenyl group" may respectively be: i) a fully deuterated C₁-C₆₀ alkyl group (or fully deuterated C₁-C₂₀ alkyl group or the like), fully deuterated C₃-C₁₀ cycloalkyl group, fully deuterated C₁-C₁₀ heterocycloalkyl group, or fully deuterated phenyl group, in which all hydrogen atoms are substituted with deuterium atoms; or ii) a partially deuterated C₁-C₆₀ alkyl group (or partially deuterated C₁-C₂₀ alkyl group or the like), partially deuterated C₃-C₁₀ cycloalkyl group, partially deuterated C₁-C₁₀ heterocycloalkyl group, or partially deuterated phenyl group, in which some of hydrogen atoms are substituted with deuterium atoms.

[0163] The "(C₁-C₂₀ alkyl)'X' group" refers to a 'X' group substituted with at least one C₁-C₂₀ alkyl group. For example, the "(C₁-C₂₀ alkyl)C₃-C₁₀ cycloalkyl group" as used herein refers to a C₃-C₁₀ cycloalkyl group substituted with at least one C₁-C₂₀ alkyl group, and the "(C₁-C₂₀ alkyl)phenyl group" as used herein refers to a phenyl group substituted with at least one C₁-C₂₀ alkyl group. Examples of the (C₁ alkyl)phenyl group may include a toluyl group.

[0164] In the present specification, "an azaindole group, an azabenzoborole group, an azabenzophosphole group, an azaindene group, an azabenzosilole group, an azabenzogermole group, an azabenzothiophene group, an azabenzoselenophene group, an azabenzofuran group, an azacarbazole group, an azadibenzoborole group, an azadibenzophosphole group, an azafluorene group, an azadibenzosilole group, an azadibenzogermole group, an azadibenzothiophene group, an azadibenzoselenophene group, an azadibenzofuran group, an azadibenzothiophene 5-oxide group, an aza-9H-fluorene-9-one group, and an azadibenzothiophene 5,5-dioxide group" each refer to a hetero ring in which at least one ring-forming carbon atom is substituted with nitrogen atom and respectively having an identical backbone as "an indole group, a benzoborole group, a benzophosphole group, an indene group, a benzosilole group, a benzogermole group, a benzothiophene group, a benzoselenophene group, a benzofuran group, a carbazole group, a dibenzoborole group, a dibenzophosphole group, a fluorene group, a dibenzosilole group, a dibenzogermole group, a dibenzothiophene group, a dibenzoselenophene group, a dibenzofuran group, a dibenzothiophene 5-oxide group, a 9H-fluorene-9-one group, and a dibenzothiophene 5,5-dioxide group".

[0165] Substituents of the substituted C₅-C₃₀ carbocyclic group, the substituted C₂-C₃₀ heterocyclic group, the substituted C₁-C₆₀ alkyl group, the substituted C₂-C₆₀ alkenyl group, the substituted C₂-C₆₀ alkynyl group, the substituted C₁-C₆₀ alkoxy group, the substituted C₃-C₁₀ cycloalkyl group, the substituted C₁-C₁₀ heterocycloalkyl group, the substituted C₃-C₁₀ cycloalkenyl group, the substituted C₂-C₁₀ heterocycloalkenyl group, the substituted C₆-C₆₀ aryl group,

the substituted C₇-C₆₀ alkyl aryl group, the substituted C₆-C₆₀ aryloxy group, the substituted C₆-C₆₀ arylthio group, the substituted C₁-C₆₀ heteroaryl group, the substituted C₂-C₆₀ alkyl heteroaryl group, the substituted monovalent non-aromatic condensed polycyclic group, and the substituted monovalent non-aromatic condensed heteropolycyclic group may each independently be:

5 deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or a C₁-C₆₀ alkoxy group;

10 a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or C₁-C₆₀ alkoxy group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, a C₃-C₁₀ cycloalkenyl group, a C₂-C₁₀ heterocycloalkenyl group, a C₆-C₆₀ aryl group, a C₇-C₆₀ alkyl aryl group, a C₆-C₆₀ aryloxy group, a C₆-C₆₀ arylthio group, a C₁-C₆₀ heteroaryl group, a C₂-C₆₀ alkyl heteroaryl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, -N(Q₁₁)(Q₁₂), -Si(Q₁₃)(Q₁₄)(Q₁₅), -B(Q₁₆)(Q₁₇), -P(=O)(Q₁₈)(Q₁₉), -P(Q₁₈)(Q₁₉), or any combination thereof; a C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, a C₃-C₁₀ cycloalkenyl group, a C₂-C₁₀ heterocycloalkenyl group, a C₆-C₆₀ aryl group, a C₇-C₆₀ alkyl aryl group, a C₆-C₆₀ aryloxy group, a C₆-C₆₀ arylthio group, a C₁-C₆₀ heteroaryl group, a C₂-C₆₀ alkyl heteroaryl group, a monovalent non-aromatic condensed polycyclic group, or a monovalent non-aromatic condensed heteropolycyclic group;

15 a C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, a C₃-C₁₀ cycloalkenyl group, a C₂-C₁₀ heterocycloalkenyl group, a C₆-C₆₀ aryl group, a C₇-C₆₀ alkyl aryl group, a C₆-C₆₀ aryloxy group, a C₆-C₆₀ arylthio group, a C₁-C₆₀ heteroaryl group, a C₂-C₆₀ alkyl heteroaryl group, a monovalent non-aromatic condensed polycyclic group, or a monovalent non-aromatic condensed heteropolycyclic group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, a C₁-C₆₀ alkoxy group, a C₃-C₁₀ cycloalkyl group, a C₁-C₁₀ heterocycloalkyl group, a C₃-C₁₀ cycloalkenyl group, a C₂-C₁₀ heterocycloalkenyl group, a C₆-C₆₀ aryl group, a C₇-C₆₀ alkyl aryl group, a C₆-C₆₀ aryloxy group, a C₆-C₆₀ arylthio group, a C₁-C₆₀ heteroaryl group, a C₂-C₆₀ alkyl heteroaryl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, -N(Q₂₁)(Q₂₂), -Si(Q₂₃)(Q₂₄)(Q₂₅), -B(Q₂₆)(Q₂₇), -P(=O)(Q₂₈)(Q₂₉), -P(Q₂₈)(Q₂₉), or any combination thereof;

20 -N(Q₃₁)(Q₃₂), -Si(Q₃₃)(Q₃₄)(Q₃₅), -B(Q₃₆)(Q₃₇), -P(=O)(Q₃₈)(Q₃₉), or -P(Q₃₈)(Q₃₉); or any combination thereof.

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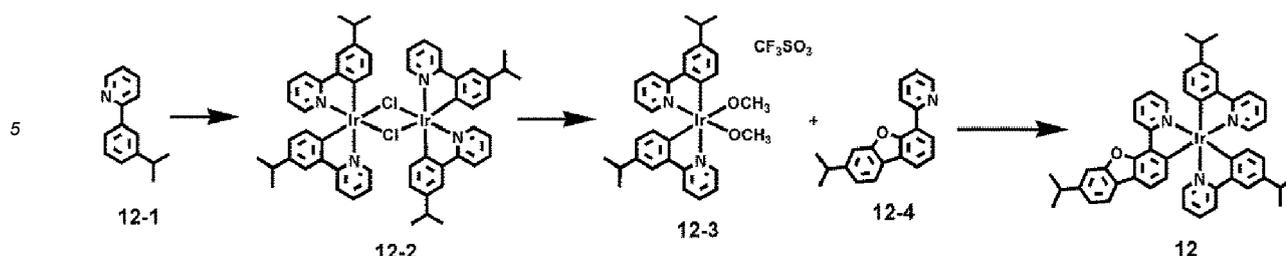
[0166] In the present specification, Q₁ to Q₉, Q₁₁ to Q₁₉, Q₂₁ to Q₂₉, and Q₃₁ to Q₃₉ may each independently be: hydrogen; deuterium; -F; -Cl; -Br; -I; a hydroxyl group; a cyano group; a nitro group; an amidino group; a hydrazine group; a hydrazone group; a carboxylic acid group or a salt thereof; a sulfonic acid group or a salt thereof; a phosphoric acid group or a salt thereof; a C₁-C₆₀ alkyl group unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof; a C₂-C₆₀ alkenyl group; a C₂-C₆₀ alkynyl group; a C₁-C₆₀ alkoxy group; a C₃-C₁₀ cycloalkyl group; a C₁-C₁₀ heterocycloalkyl group; a C₃-C₁₀ cycloalkenyl group; a C₂-C₁₀ heterocycloalkenyl group; a C₆-C₆₀ aryl group unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof; a C₆-C₆₀ aryloxy group; a C₆-C₆₀ arylthio group; a C₁-C₆₀ heteroaryl group; a monovalent non-aromatic condensed polycyclic group; or a monovalent non-aromatic condensed heteropolycyclic group.

[0167] Hereinafter, a compound and an organic light-emitting device according to an embodiment will be described in detail with reference to Synthesis Examples and Examples, however, the present disclosure is not limited thereto. The wording "B was used instead of A" used in describing Synthesis Examples means that an amount of B used was identical to an amount of A used based on molar equivalence.

Examples

Synthesis Example 1 (Compound 12)

[0168]



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Synthesis of Compound 12-2

[0169] 2.2 grams (g) (6.24 mmol) of IrCl_3 hydrate and 2.71 g (3 eq., 15.31 mmol) of Compound 12-1 were added to a flask, followed by mixing with 24 milliliters (mL) of 2-ethoxyethanol and 8 mL of H_2O . Then, in N_2 atmosphere, the mixture was stirred under reflux at a temperature of 120°C for 18 hours. The resulting product was cooled to room temperature to obtain a precipitate. The precipitate was filtered and washed sequentially with water, methanol, and hexane, followed by drying, to thereby obtaining 2.6 g of Compound 12-2. Compound 12-2 was used in the next step without any further purification.

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Synthesis of Compound 12-3

[0170] 2.5 g (1.56 mmol) of Compound 12-2 was mixed with 30 mL of dichloromethane, followed by slowly adding dropwise a mixture of 0.92 g (2.3 eq., 3.59 mmol) of AgOTf and 10 mL of methanol. Upon blocking out light, the obtained product was stirred overnight at room temperature to produce a resulting product, which was then filtered using a celite filter. The filtrate was concentrated to yield 3.2 g of Compound 12-3 which was used in the next step without any further purification.

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Synthesis of Compound 12

[0171] 3 g (3.77 mmol) of Compound 12-3 and 1.3 g (1.2 eq., 4.52 mmol) of Compound 12-4 were mixed with 20 mL of ethanol, followed by stirring under reflux at a temperature of 90°C overnight. Once the reaction was complete, the product was cooled to room temperature and filtered to obtain a solid. The resulting solid was washed with ethanol and dried to obtain the resulting product. The resulting product was dissolved in dichloromethane and purified through column chromatography to thereby obtain 1.1 g of Compound 12.

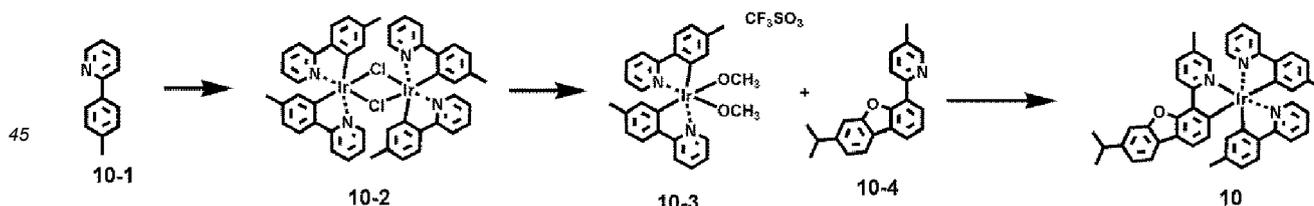
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LCMS : m/z calcd for $\text{C}_{48}\text{H}_{44}\text{IrN}_3\text{O}$, 871.1; Found 871.31

Synthesis Example 2 (Compound 10)

[0172]

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Synthesis of Compound 10-2

[0173] 2.8 g (7.94 mmol) of IrCl_3 hydrate and 3.0 g (2.23 eq., 17.71 mmol) of Compound 10-1 were added to a flask, followed by mixing with 30 mL of 2-ethoxyethanol and 10 mL of H_2O . Then, in N_2 atmosphere, the mixture was stirred under reflux at a temperature of 120°C for 18 hours. The resulting product was cooled to room temperature to obtain a precipitate. The precipitate was filtered and washed sequentially with water, methanol, and hexane, followed by drying, to thereby obtaining 4.0 g of Compound 10-2. Compound 10-2 was used in the next step without any further purification.

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Synthesis of Compound 10-3

[0174] 2.0 g (1.25 mmol) of Compound 10-2 was mixed with 30 mL of dichloromethane, followed by slowly adding dropwise a mixture of 0.74 g (2.3 eq., 2.87 mmol) of AgOTf and 10 mL of methanol. Upon blocking out light, the obtained product was stirred overnight at room temperature to produce a resulting product, which was then filtered using a celite filter. Then, the filtrate was concentrated to obtain 2.5 g of Compound 10-3. Compound 10-3 was used in the next step without any further purification.

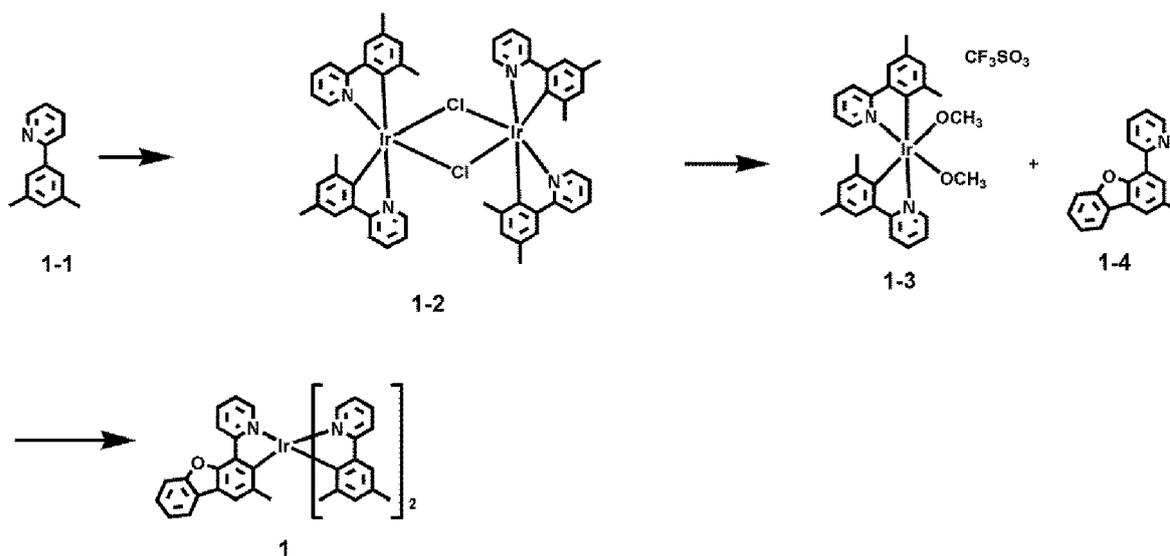
Synthesis of Compound 10

[0175] 2.4 g (3.24 mmol) of Compound 10-3 and 1.17 g (1.2 eq., 3.89 mmol) of Compound 10-4 were mixed with 20 mL of ethanol, followed by stirring under reflux at a temperature of 90 °C overnight. Once the reaction was complete, the product was cooled to room temperature and filtered to obtain a solid. The resulting solid was washed with ethanol and dried to obtain a resulting product. The resulting product was dissolved in dichloromethane and purified through column chromatography to thereby obtain 0.8 g of Compound 10.

LCMS : m/z calcd for C₄₅H₃₈IrN₃O, 829.26; Found 830.29

Synthesis Example 3 (Compound 1)

[0176]



Synthesis of Compound 1-2

[0177] Compound 1-2 was synthesized in substantially the same manner as in Synthesis of Compound 1-2 in Synthesis Example 1, except that Compound 1-1 was used instead of Compound 12-1.

Synthesis of Compound 1-3

[0178] Compound 1-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 1-2 was used instead of Compound 12-2.

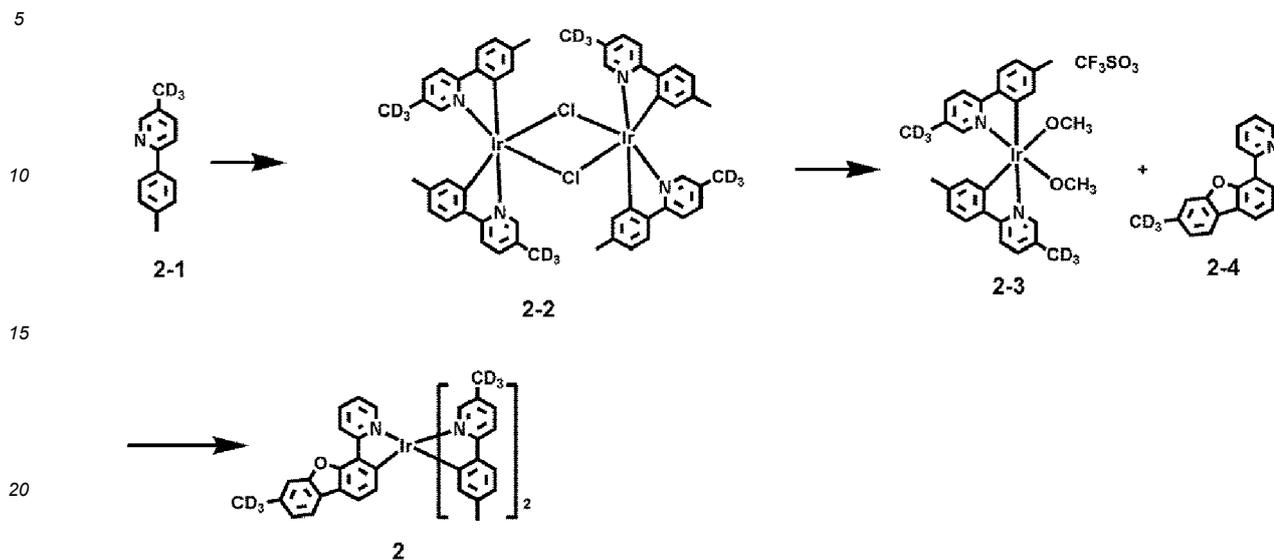
Synthesis of Compound 1

[0179] Compound 1 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 1-3 and Compound 1-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 11%).

LCMS : m/z calcd for C₄₄H₃₆IrN₃O, 814.99; Found 815.25

Synthesis Example 4 (Compound 2)

[0180]



Synthesis of Compound 2-2

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[0181] Compound 2-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 2-1 was used instead of Compound 12-1.

Synthesis of Compound 2-3

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[0182] Compound 2-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 2-2 was used instead of Compound 12-2.

Synthesis of Compound 2

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[0183] Compound 2 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 2-3 and Compound 2-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 60%).

LCMS : m/z calcd for C₄₄H₂₇D₉IrN₃O, 824.05; Found 824.31

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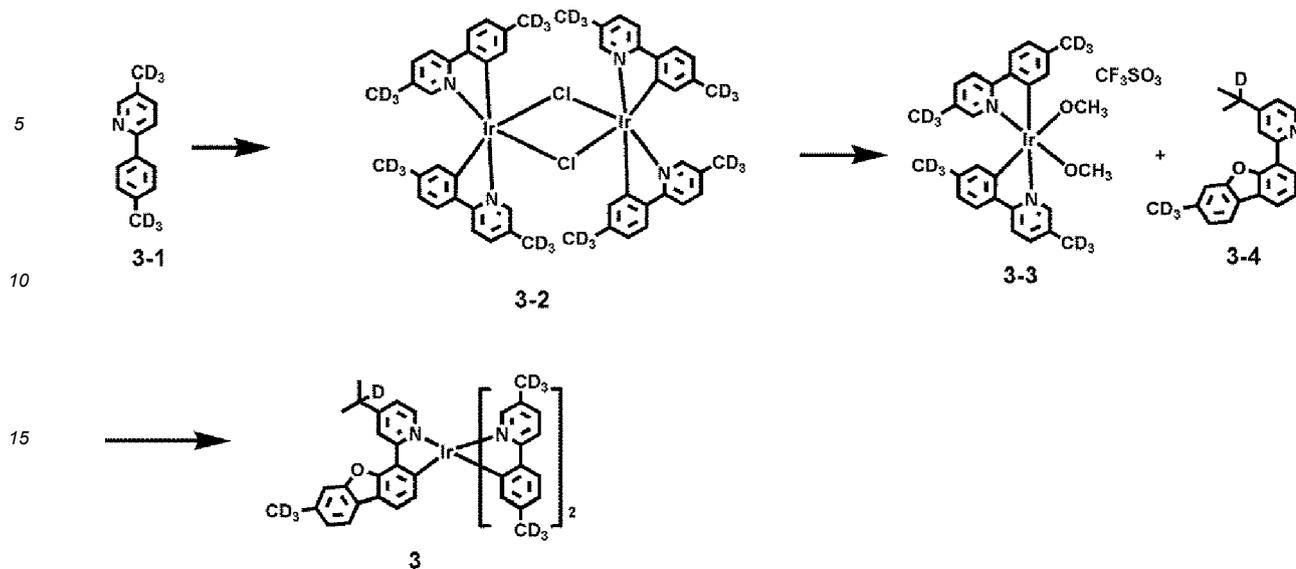
Synthesis Example 5 (Compound 3)

[0184]

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Synthesis of Compound 3-2

[0185] Compound 3-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 3-1 was used instead of Compound 12-1.

Synthesis of Compound 3-3

[0186] Compound 3-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 3-2 was used instead of Compound 12-2.

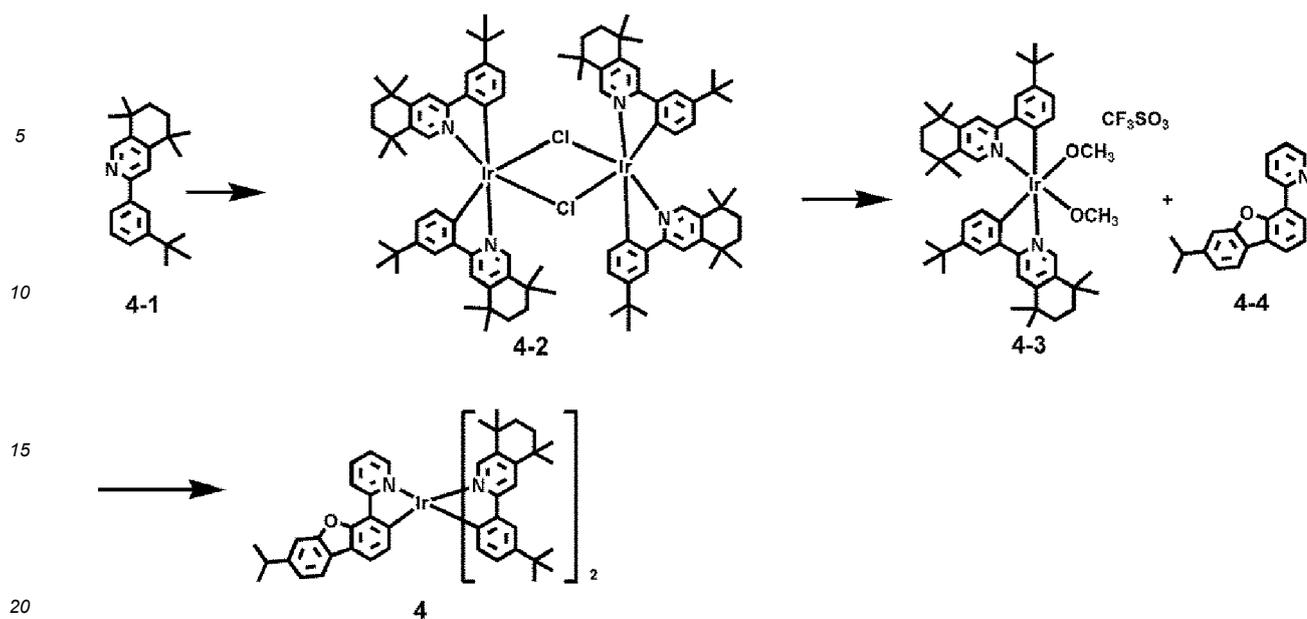
Synthesis of Compound 3

[0187] Compound 3 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 3-3 and Compound 3-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 58%).

LCMS : m/z calcd for $C_{47}H_{26}D_{16}IrN_3O$, 873.17; Found 873.40

Synthesis Example 6 (Compound 4)

[0188]



Synthesis of Compound 4-2

25 **[0189]** Compound 4-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 4-1 was used instead of Compound 12-1.

Synthesis of Compound 4-3

30 **[0190]** Compound 4-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 4-2 was used instead of Compound 12-2.

Synthesis of Compound 4

35 **[0191]** Compound 4 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 4-3 and Compound 4-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 62%).

LCMS : m/z calcd for $C_{66}H_{76}IrN_3O$, 1117.56; Found 1119.56

Synthesis Example 7 (Compound 5)

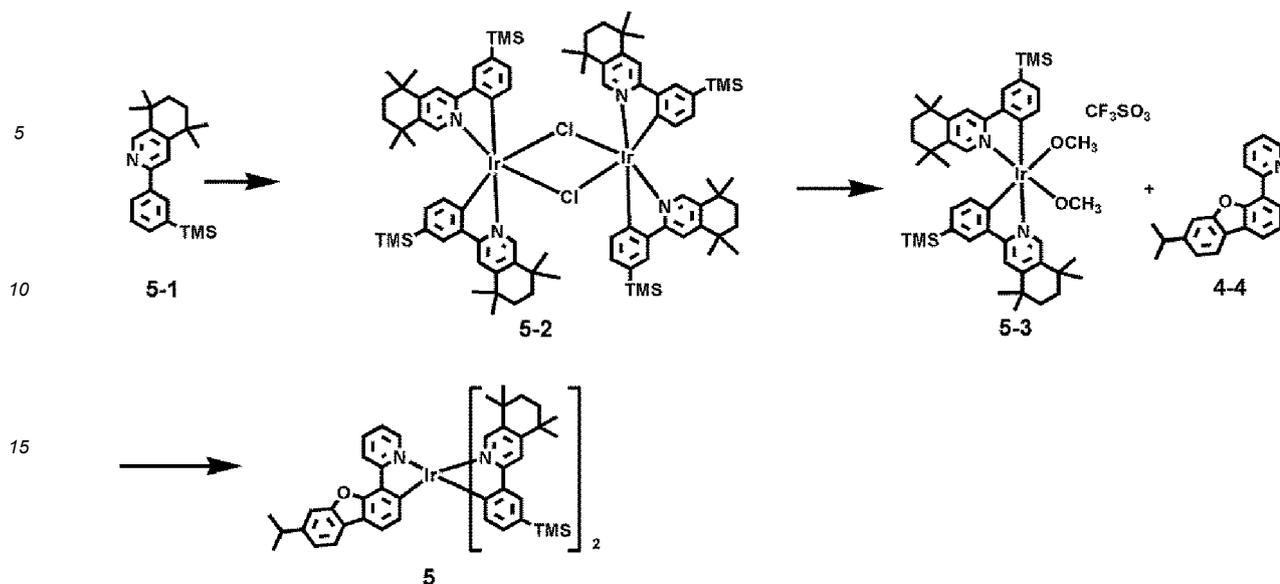
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[0192]

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Synthesis of Compound 5-2

[0193] Compound 5-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 5-1 was used instead of Compound 12-1.

Synthesis of Compound 5-3

[0194] Compound 5-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 5-2 was used instead of Compound 12-2.

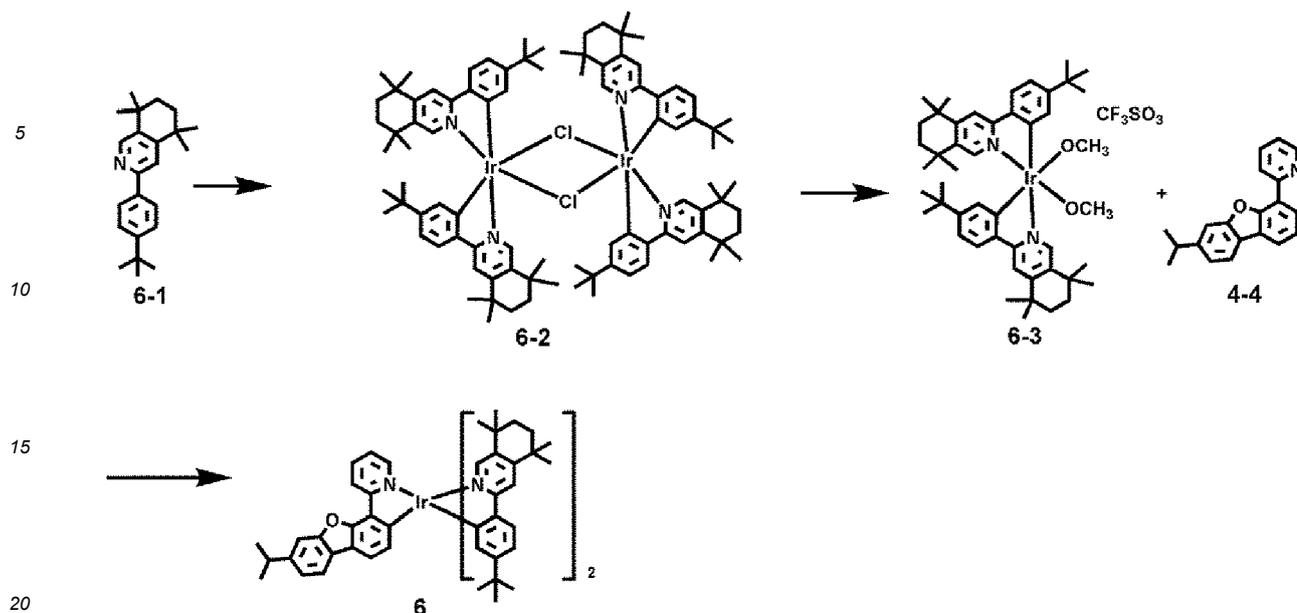
Synthesis of Compound 5

[0195] Compound 5 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 5-3 and Compound 4-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 48%).

LCMS : m/z calcd for $C_{64}H_{76}IrN_3OSi_2$, 1151.52; Found 1151.7

Synthesis Example 8 (Compound 6)

[0196]



Synthesis of Compound 6-2

25 **[0197]** Compound 6-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 6-1 was used instead of Compound 12-1.

Synthesis of Compound 6-3

30 **[0198]** Compound 6-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 6-2 was used instead of Compound 12-2.

Synthesis of Compound 6

35 **[0199]** Compound 6 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 6-3 and Compound 4-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 56%).

LCMS : m/z calcd for $C_{66}H_{76}IrN_3O$, 1119.55; Found 1119.56

Synthesis Example 9 (Compound 7)

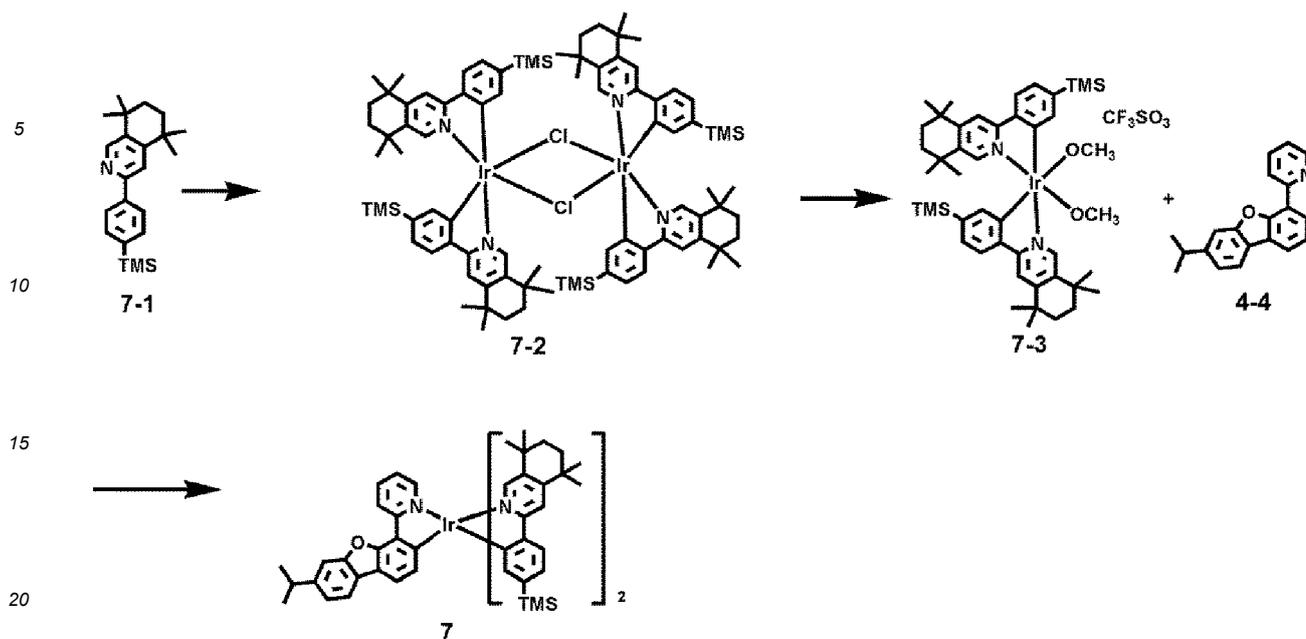
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[0200]

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Synthesis of Compound 7-2

25 **[0201]** Compound 7-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 7-1 was used instead of Compound 12-1.

Synthesis of Compound 7-3

30 **[0202]** Compound 7-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 7-2 was used instead of Compound 12-2.

Synthesis of Compound 7

35 **[0203]** Compound 7 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 7-3 and Compound 4-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 49%).

LCMS : m/z calcd for $C_{64}H_{76}IrN_3OSi_2$, 1151.52; Found 1151.7

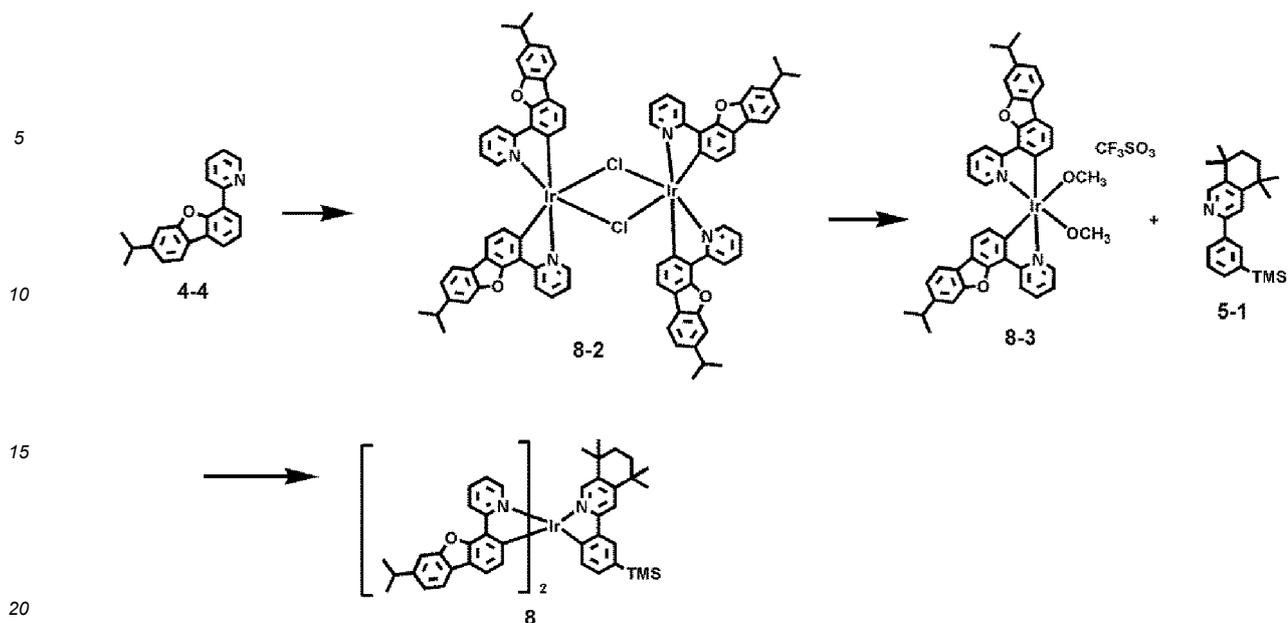
40 Synthesis Example 10 (Compound 8)

[0204]

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Synthesis of Compound 8-2

25 **[0205]** Compound 8-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 4-4 was used instead of Compound 12-1.

Synthesis of Compound 8-3

30 **[0206]** Compound 8-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 8-2 was used instead of Compound 12-2.

Synthesis of Compound 8

35 **[0207]** Compound 8 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 8-3 and Compound 5-1 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 50%).

LCMS : m/z calcd for $C_{62}H_{62}IrN_3O_2Si$, 1101.42; Found 1101.48

Synthesis Example 11 (Compound 9)

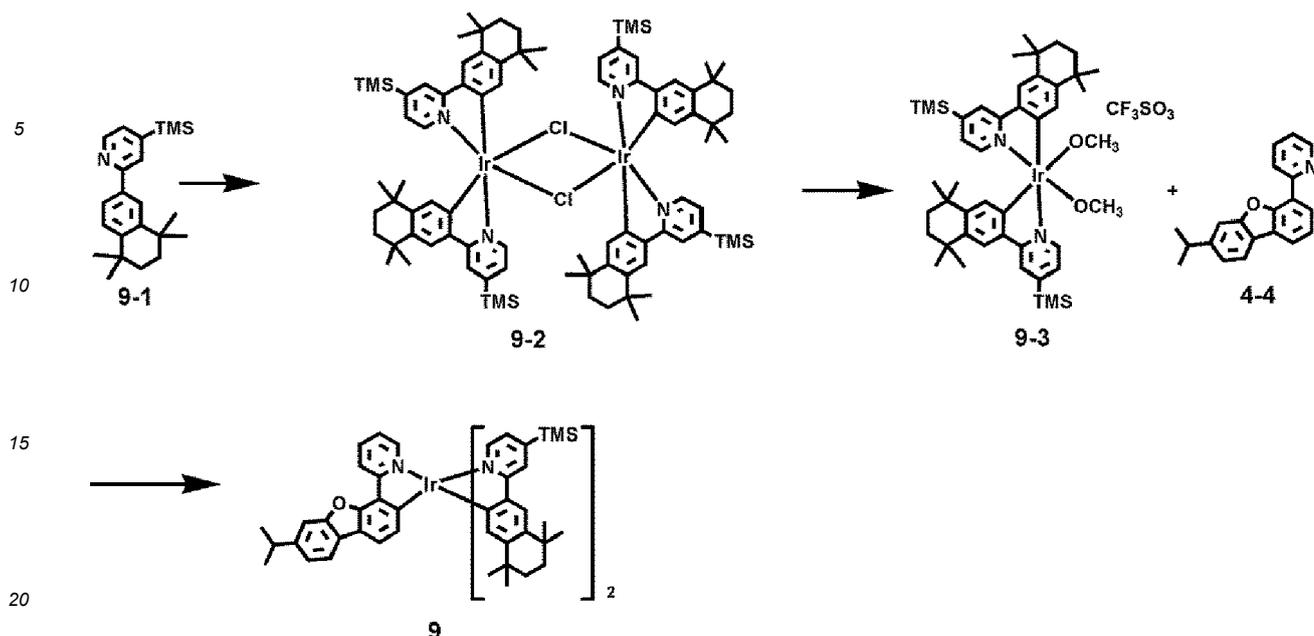
40

[0208]

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Synthesis of Compound 9-2

25 **[0209]** Compound 9-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 9-1 was used instead of Compound 12-1.

Synthesis of Compound 9-3

30 **[0210]** Compound 9-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 9-2 was used instead of Compound 12-2.

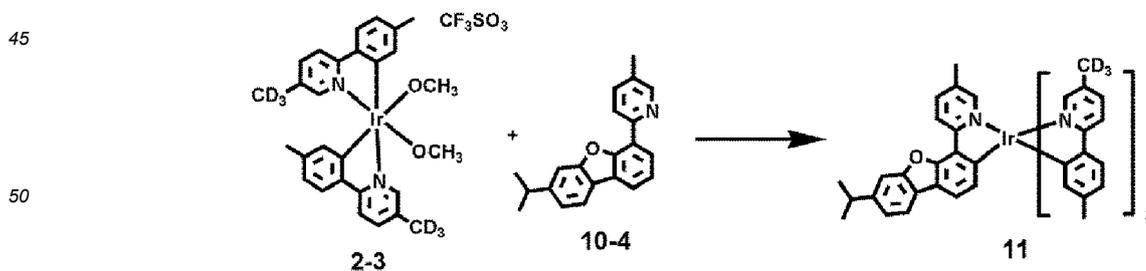
Synthesis of Compound 9

35 **[0211]** Compound 9 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 9-3 and Compound 4-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 48%).

LCMS : m/z calcd for $C_{64}H_{76}IrN_3OSi_2$, 1151.52; Found 1151.7

40 Synthesis Example 12 (Compound 11)

[0212]

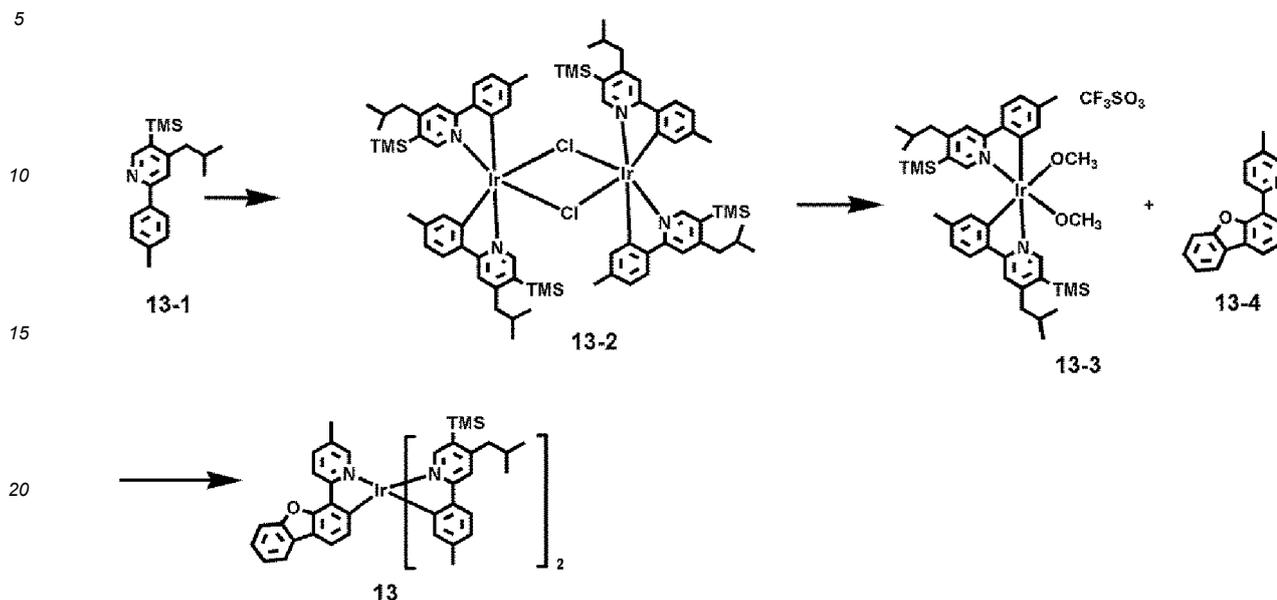


55 **[0213]** Compound 11 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 2-3 and Compound 10-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 63%).

LCMS : m/z calcd for $C_{47}H_{36}D_6IrN_3O$, 863.11; Found 863.33

Synthesis Example 13 (Compound 13)

[0214]



25 Synthesis of Compound 13-2

[0215] Compound 13-2 was synthesized in substantially the same manner as in Synthesis of Compound 12-2 in Synthesis Example 1, except that Compound 13-1 was used instead of Compound 12-1.

30 Synthesis of Compound 13-3

[0216] Compound 13-3 was synthesized in substantially the same manner as in Synthesis of Compound 12-3 in Synthesis Example 1, except that Compound 13-2 was used instead of Compound 12-2.

35 Synthesis of Compound 13

[0217] Compound 13 was synthesized in substantially the same manner as in Synthesis of Compound 12 in Synthesis Example 1, except that Compound 13-3 and Compound 13-4 were used instead of Compound 12-3 and Compound 12-4, respectively (yield: 54%).

40 LCMS : m/z calcd for $C_{56}H_{64}IrN_3OSi_2$, 1043.42; Found 1043.51

Example 1

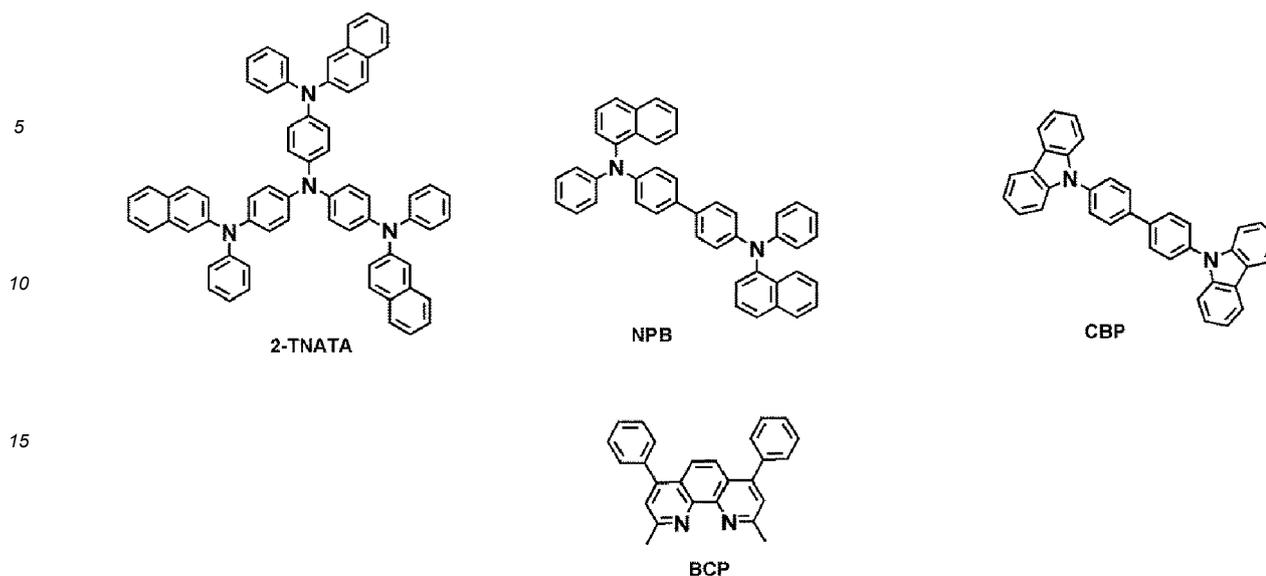
45 [0218] A glass substrate, on which an anode having an ITO/Ag/ITO (70 Å/1,000 Å/70 Å) structure was deposited, was cut to a size of 50 millimeters (mm) × 50 mm × 0.5 mm, sonicated in isopropyl alcohol and water for 5 minutes each, and cleaned by exposure to ultraviolet rays and ozone for 30 minutes. Subsequently, the glass substrate was mounted on a vacuum-deposition device.

[0219] 2-TNATA was vacuum-deposited on the anode to form a hole injection layer having a thickness of 600 Å, and 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (hereinafter, referred as "NPB") was vacuum-deposited on the hole injection layer to form a hole transport layer having a thickness of 1,350 Å.

50 [0220] Subsequently, CBP (host) and Compound 1 (dopant) were co-deposited on the hole transport layer at a weight ratio of 98:2 to form an emission layer having a thickness of 400 Å.

[0221] Then, BCP was vacuum-deposited on the emission layer to form a hole blocking layer having a thickness of 50 Å. Alq₃ was vacuum-deposited on the hole blocking layer to form an electron transport layer having a thickness of 350 Å. LiF was vacuum-deposited on the electron transport layer to form an electron injection layer having a thickness of 10 Å. Mg and Ag were co-deposited on the electron injection layer at a weight ratio of 90:10 to form a cathode having a thickness of 120 Å, thereby completing the manufacture of an organic light-emitting device.

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Examples 2 to 13 and Comparative Examples A, B, and C

[0222] Organic light-emitting devices were manufactured in substantially the same manner as in Example 1, except that the compounds shown in Table 2 were used instead of Compound 1 as a dopant in the formation of an emission layer.

Evaluation Example 2: Evaluation of characteristics of organic light-emitting device

[0223] The driving voltage, maximum value of external quantum efficiency (Max EQE), roll-off ratio, maximum emission wavelength of electroluminescence (EL) spectrum, and lifespan (LT_{97}) of each organic light-emitting device manufactured in Examples 1 to 13 and Comparative Examples A, B, and C were evaluated. The results thereof are shown in Table 2. A Keithley 2400 current voltmeter and a luminance meter (Minolta Cs-1000A) were used in the evaluation. The lifespan (LT_{97}) refers to time required for the initial luminance of 3,500 nit of the organic light-emitting device to reduce by 97 %. The roll-off ratio was calculated by Equation 20:

Equation 20

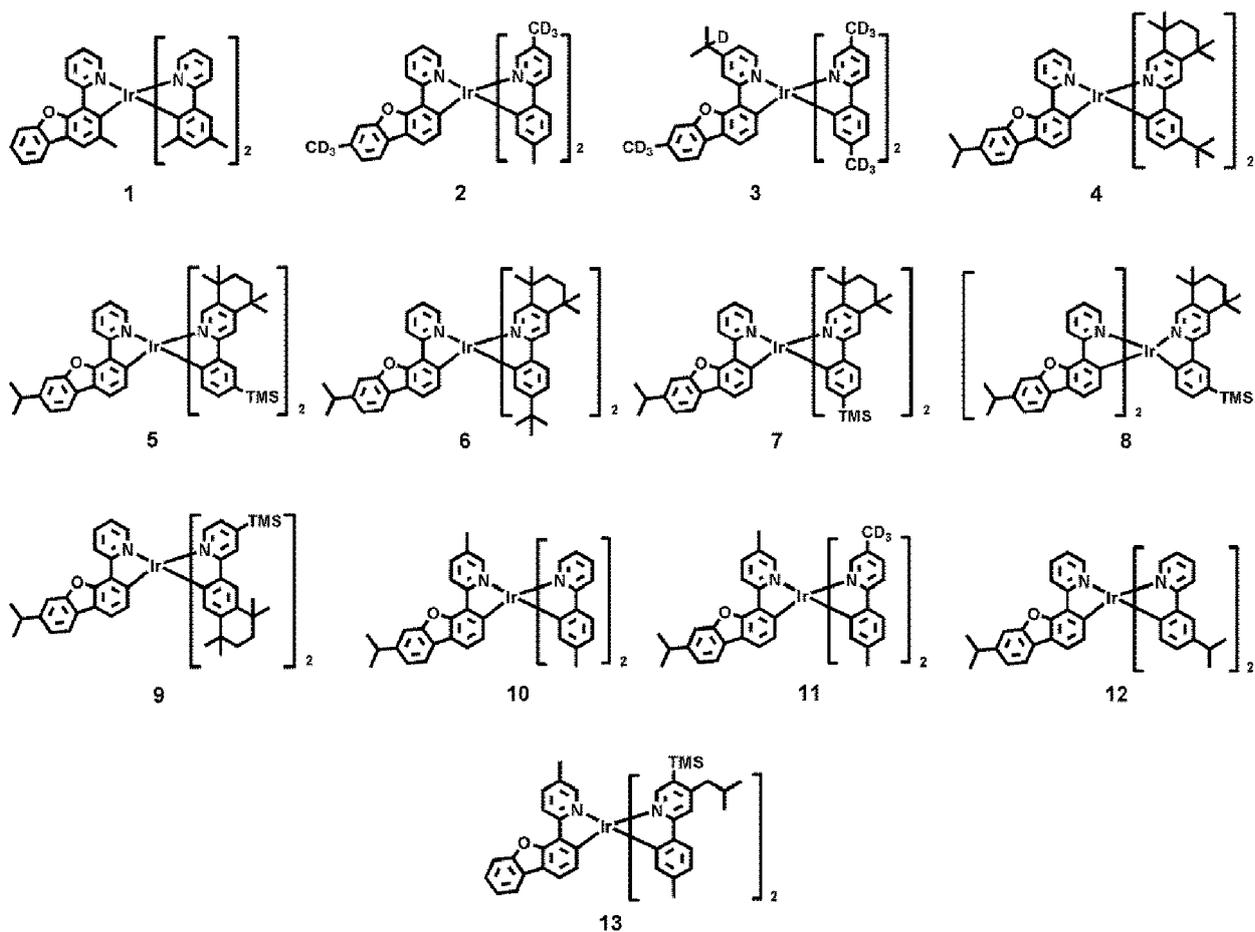
$$\text{Roll-off ratio} = \{1 - (\text{efficiency (at 3,500 nit)} / \text{maximum luminescence efficiency})\} \times 100 \%$$

Table 2

	Dopant in emission layer Compound No.	Driving voltage (V)	Max EQE (%)	Roll- off ratio (%)	Maximum emission wavelength (nm)	LT_{97} (hr) (at 3500 nit)
Example 1	1	4.74	22.2	10	533	165
Example 2	2	4.63	20.3	9	535	157
Example 3	3	4.59	20.4	7	531	159
Example 4	4	4.56	21.1	4	539	161
Example 5	5	4.62	21.5	5	537	163
Example 6	6	4.60	20.8	7	538	158
Example 7	7	4.50	22.1	8	535	157

(continued)

	Dopant in emission layer Compound No.	Driving voltage (V)	Max EQE (%)	Roll- off ratio (%)	Maximum emission wavelength (nm)	LT ₉₇ (hr) (at 3500 nit)	
5	Example 8	8	4.66	22.4	8	534	160
	Example 9	9	4.65	20.8	7	535	150
10	Example 10	10	4.60	21.6	7	528	162
	Example 11	11	4.66	22.5	9	524	155
	Example 12	12	4.51	20.9	10	531	165
15	Example 13	13	4.72	21.8	8	527	151
	Comparative Example A	A	5.8	16.1	18	531	134
	Comparative Example B	B	5.6	15.2	16	534	146
20	Comparative Example C	C	5.4	15.8	10	529	120



Y₁₁ is N, and Y₁₂ is C,

ring CY₁ and ring CY₁₁ are each independently a C₁-C₃₀ heterocyclic group,

ring CY₂ and ring CY₁₂ are each independently a C₅-C₃₀ carbocyclic group or a C₁-C₃₀ heterocyclic group,

X₂₁ is O, S, Se, N(R₂₈), C(R₂₈)(R₂₉), or Si(R₂₈)(R₂₉),

R₁, R₂, R₂₈, R₂₉, Z₁, and Z₂ are each independently deuterium, -F, -Cl, -Br, -I, -SF₅, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C₁-C₆₀ alkyl group, a substituted or unsubstituted C₂-C₆₀ alkenyl group, a substituted or unsubstituted C₂-C₆₀ alkynyl group, a substituted or unsubstituted C₁-C₆₀ alkoxy group, a substituted or unsubstituted C₆-C₃₀ unsaturated carbocyclic group, a substituted or unsubstituted C₂-C₃₀ unsaturated heterocyclic group, -N(Q₁)(Q₂), -Si(Q₃)(Q₄)(Q₅), -Ge(Q₃)(Q₄)(Q₅), -B(Q₆)(Q₇), -P(=O)(Q₈)(Q₉), or -P(Q₈)(Q₉),

a₁, a₂, and d₁ are each independently an integer from 0 to 10, wherein, when a₁ is 2 or greater, at least two R₁(s) are identical to or different from each other; when a₂ is 2 or greater, at least two R₂(s) are identical to or different from each other; and when d₁ is 2 or greater, at least two Z₁(s) are identical to or different from each other,

d₂ is an integer from 1 to 10, wherein, when d₂ is 2 or greater, at least two Z₂(s) are identical to or different from each other,

at least two selected from a plurality of R₁(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from a plurality of R₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from a plurality of Z₁(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from a plurality of Z₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

at least two selected from R₁(s), R₂(s), Z₁(s), and Z₂(s) are optionally linked to form a C₅-C₃₀ carbocyclic group unsubstituted or substituted with at least one R_{10a} or a C₁-C₃₀ heterocyclic group unsubstituted or substituted with at least one R_{10a},

R_{10a} is understood by referring to the description of R₁ provided herein,

* and *' each indicate a binding site to M in Formula 1, and

a substituent of the substituted C₁-C₆₀ alkyl group, the substituted C₂-C₆₀ alkenyl group, the substituted C₂-C₆₀ alkynyl group, the substituted C₁-C₆₀ alkoxy group, the substituted C₆-C₃₀ unsaturated carbocyclic group, and the substituted C₂-C₃₀ unsaturated heterocyclic group is:

deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or a C₁-C₆₀ alkoxy group;

a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, or a C₁-C₆₀ alkoxy group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₆-C₃₀ unsaturated carbocyclic group, a C₂-C₃₀ unsaturated heterocyclic group, -N(Q₁₁)(Q₁₂), -Si(Q₁₃)(Q₁₄)(Q₁₅), -Ge(Q₁₃)(Q₁₄)(Q₁₅), -B(Q₁₆)(Q₁₇), -P(=O)(Q₁₈)(Q₁₉), -P(Q₁₈)(Q₁₉), or any combination thereof;

a C₆-C₃₀ unsaturated carbocyclic group or a C₂-C₃₀ unsaturated heterocyclic group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₆₀ alkyl group, a C₂-C₆₀ alkenyl group, a C₂-C₆₀ alkynyl group, a C₁-C₆₀ alkoxy group, a C₆-C₃₀ unsaturated carbocyclic group, a C₂-C₃₀ unsaturated heterocyclic group, -N(Q₂₁)(Q₂₂), -Si(Q₂₃)(Q₂₄)(Q₂₅), -Ge(Q₂₃)(Q₂₄)(Q₂₅), -B(Q₂₆)(Q₂₇), -P(=O)(Q₂₈)(Q₂₉), -P(Q₂₈)(Q₂₉), or any combination thereof;

-N(Q₃₁)(Q₃₂), -Si(Q₃₃)(Q₃₄)(Q₃₅), -Ge(Q₃₃)(Q₃₄)(Q₃₅), -B(Q₃₆)(Q₃₇), -P(=O)(Q₃₈)(Q₃₉), or -P(Q₃₈)(Q₃₉); or any combination thereof,

wherein Q₁ to Q₉, Q₁₁ to Q₁₉, Q₂₁ to Q₂₉, and Q₃₁ to Q₃₉ are each independently: hydrogen; deuterium; -F; -Cl; -Br; -I; a hydroxyl group; a cyano group; a nitro group; an amidino group; a hydrazine group; a hydrazone group; a carboxylic acid group or a salt thereof; a sulfonic acid group or a salt thereof; a phosphoric acid group or a salt thereof; a C₁-C₆₀ alkyl group unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof; a C₂-C₆₀ alkenyl group; a C₂-C₆₀ alkynyl group; a C₁-C₆₀ alkoxy group; or a C₆-C₃₀ unsaturated carbocyclic group or C₂-C₃₀ unsaturated heterocyclic group, each unsubstituted or substituted with deuterium, a C₁-C₆₀ alkyl group, a C₆-C₆₀ aryl group, or any combination thereof.

2. The organometallic compound of claim 1, wherein M is Ir; and/or wherein X₂₁ is O or S

3. The organometallic compound of claims 1 or 2, wherein

ring CY₁ and ring CY₁₁ are each independently a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group, and ring CY₂ and ring CY₁₂ are each independently a benzene group, a naphthalene group, an anthracene group, a phenanthrene group, a triphenylene group, a pyrene group, a chrysene group, a 1,2,3,4-tetrahydronaphthalene group, a thiophene group, a furan group, an indole group, a borole group, a silole group, a germole group, a phosphole group, a selenophene group, a benzoborole group, a benzophosphole group, an indene group, a benzosilole group, a benzogermole group, a benzothiophene group, a benzoselenophene group, a benzofuran group, a carbazole group, a dibenzoborole group, a dibenzophosphole group, a fluorene group, a dibenzosilole group, a dibenzogermole group, a dibenzothiophene group, a dibenzoselenophene group, a dibenzofuran group, a dibenzothiophene 5-oxide group, a 9H-fluorene-9-one group, a dibenzothiophene 5,5-dioxide group, a pyridine group, a pyrimidine group, a pyrazine group, a pyridazine group, a triazine group, a quinoline group, an isoquinoline group, a quinoxaline group, a quinazoline group, a phenanthroline group, a 5,6,7,8-tetrahydroisoquinoline group, or a 5,6,7,8-tetrahydroquinoline group.

4. The organometallic compound of any of claims 1-3, wherein R₁, R₂, R₂₈, R₂₉, Z₁, and Z₂ are each independently:

deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, -SF₅, a C₁-C₂₀ alkyl group, a C₁-C₂₀ alkenyl group, or a C₁-C₂₀ alkoxy group;

a C₁-C₂₀ alkyl group, a C₁-C₂₀ alkenyl group, or a C₁-C₂₀ alkoxy group, each substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₁₀ alkyl group, a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, or any combination thereof;

a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzimidazolyl group, a benzofuran group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuran group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, an imidazopyrimidinyl group, an azacarbazolyl group, an azadibenzofuran group, or an azadibenzothiophenyl group, each unsubstituted or substituted with deuterium, -F, -Cl, -Br, -I, -CD₃, -CD₂H, -CDH₂, -CF₃, -CF₂H, -CFH₂, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C₁-C₂₀ alkyl group, a deuterated C₂-C₂₀ alkyl group, a C₁-C₂₀ alkoxy group, a phenyl group, a (C₁-C₂₀ alkyl)phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl

group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazoliny group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, an imidazopyrimidinyl group, an azacarbazolyl group, an azadibenzofuranyl group, an azadibenzothiophenyl group, or any combination thereof; or

-N(Q₁)(Q₂), -Si(Q₃)(Q₄)(Q₅), -Ge(Q₃)(Q₄)(Q₅), -B(Q₆)(Q₇), -P(=O)(Q₈)(Q₉), or -P(Q₈)(Q₉), wherein Q₁ to Q₉ are each independently:

deuterium, -F, -CH₃, -CD₃, -CD₂H, -CDH₂, -CH₂CH₃, -CH₂CD₃, -CH₂CD₂H, -CH₂CDH₂, -CHDCH₃, -CHDCD₂H, -CHDCDH₂, -CHDCD₃, -CD₂CD₃, -CD₂CD₂H, -CD₂CDH₂, -CF₃, -CF₂H, -CFH₂, -CH₂CF₃, -CH₂CF₂H, -CH₂CFH₂, -CHFCH₃, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CHFCH₂H, -CF₂CF₃, -CF₂CF₂H, or -CF₂CFH₂; or an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an isobutyl group, a tert-butyl group, an n-pentyl group, a tert-pentyl group, a neopentyl group, an isopentyl group, a sec-pentyl group, a 3-pentyl group, a sec-isopentyl group, a phenyl group, a biphenyl group, or a naphthyl group, each unsubstituted or substituted with deuterium, -F, a C₁-C₁₀ alkyl group, a phenyl group, or any combination thereof.

5. The organometallic compound of any of claims 1-4, wherein

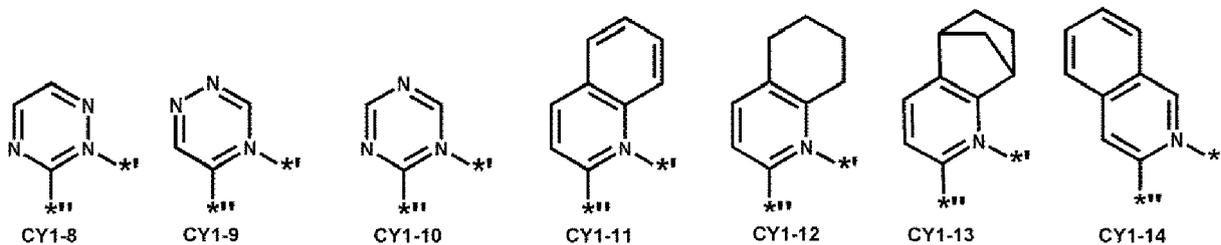
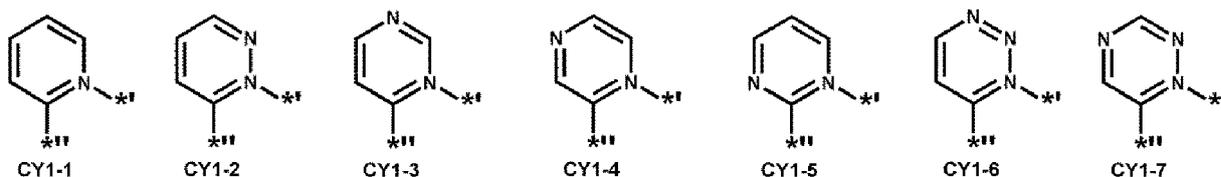
- i) a1 is 0, and a2 is 1 or 2,
- ii) a1 is 1 or 2, and a2 is 0, or
- iii) a1 is 1 or 2, and a2 is 1 or 2.

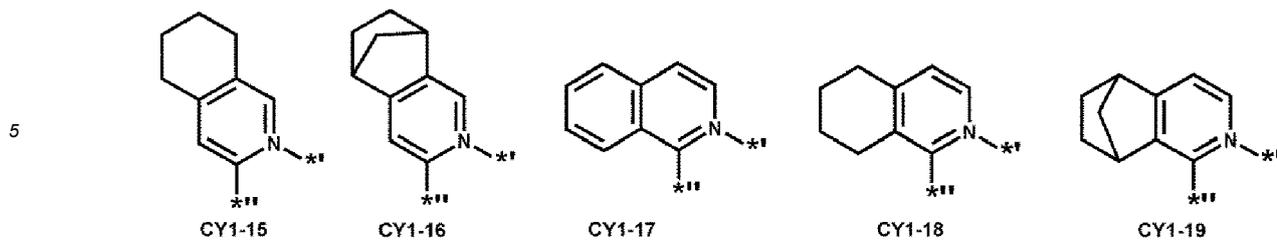
6. The organometallic compound of any of claims 1-5, wherein

d1 is 0, 1, or 2, and
d2 is 1, 2, 3, or 4.

7. The organometallic compound of any of claims 1-6 comprising at least one deuterium; and/or comprising a group represented by -Si(Q₃)(Q₄)(Q₅), a group represented by -Ge(Q₃)(Q₄)(Q₅), or any combination thereof.

8. The organometallic compound of any of claims 1-7, wherein ring CY₁ in Formula 2 is represented by one of Formulae CY1-1 to CY1-19:

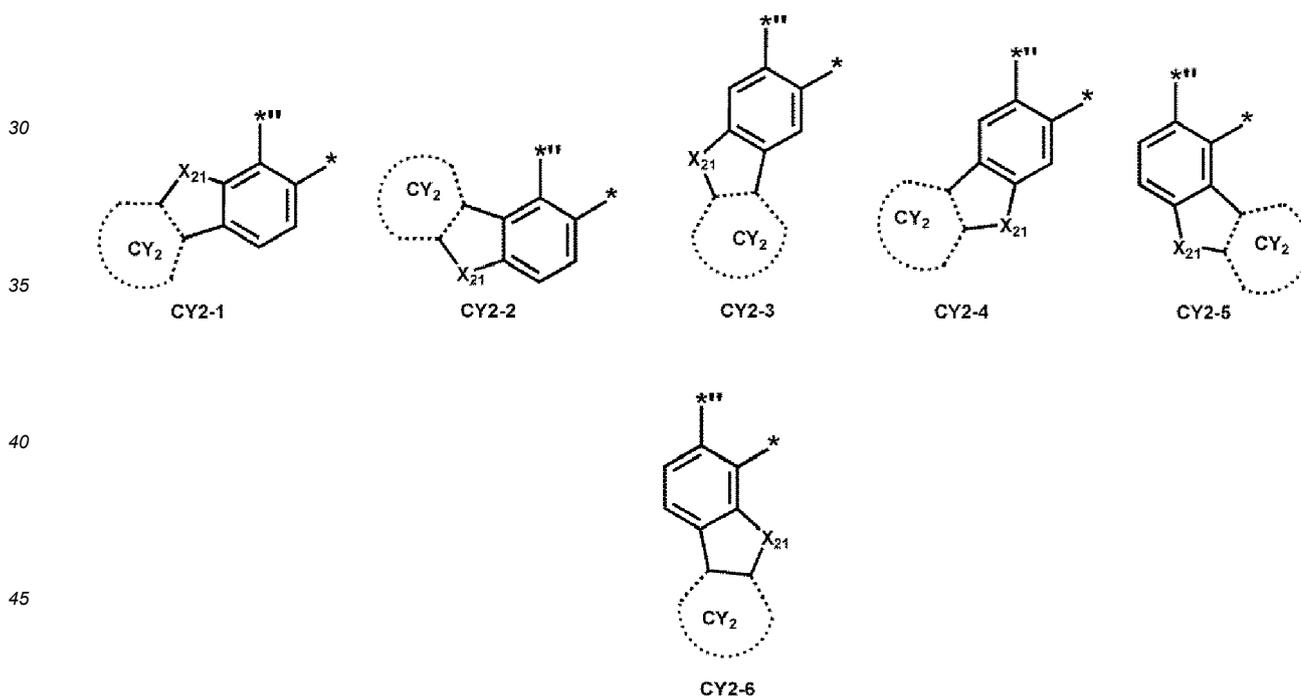




10 wherein, in Formulae CY1-1 to CY1-19, * indicates a binding site to M in Formula 1, and ** indicates a binding site to an adjacent benzo group; and/or wherein a group represented by



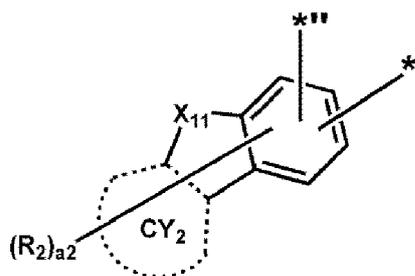
25 in Formula 2 is represented by one of Formulae CY2-1 to CY2-6:



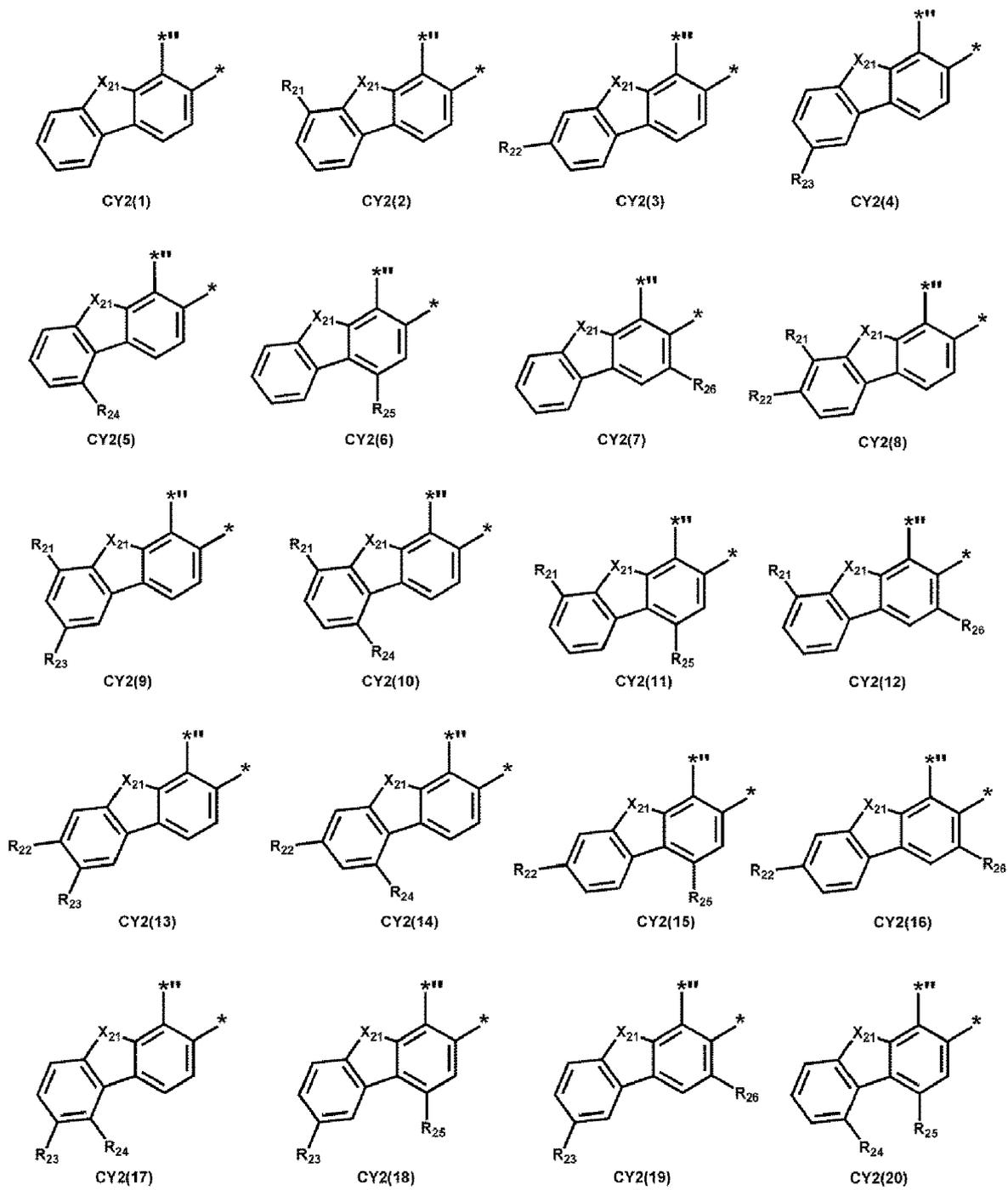
50 wherein, in Formulae CY2-1 to CY2-6, X₂₁ and ring CY₂ are each understood by referring to the descriptions thereof in claim 1, * indicates a binding site to M in Formula 1, and ** indicates a binding site to ring CY₁ in Formula 2.

9. The organometallic compound of any of claims 1-8, wherein a group represented by

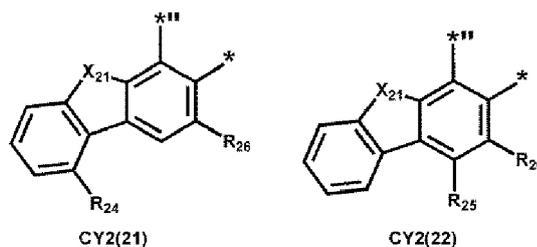
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in Formula 2 is represented by one of Formulae CY2(1) to CY2(22):



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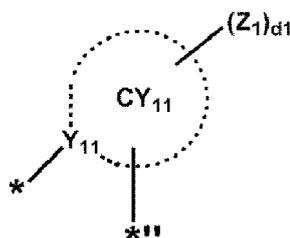
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wherein, in Formulae CY2(1) to CY2(22), X_{21} is understood by referring to the description thereof in claim 1, R_{21} to R_{26} are each understood by referring to the description of R_2 in claim 1, * indicates a binding site to M in Formula 1, and ** indicates a binding site to ring CY_1 in Formula 2.

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10. The organometallic compound of any of claims 1-9, wherein a group represented by

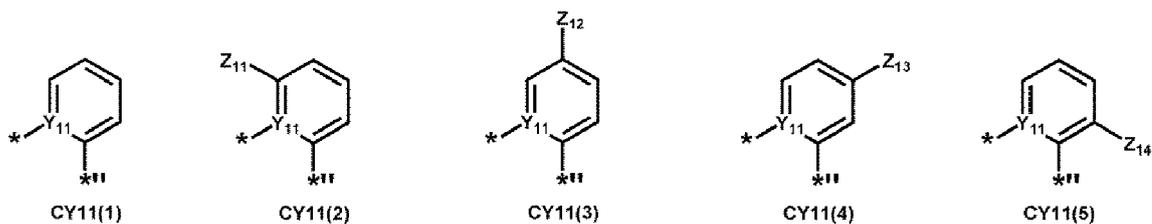
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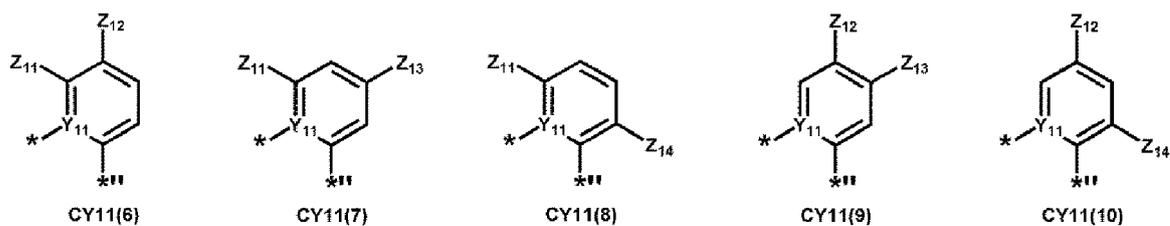
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in Formula 3 is represented by one of Formulae CY11(1) to CY11(18):

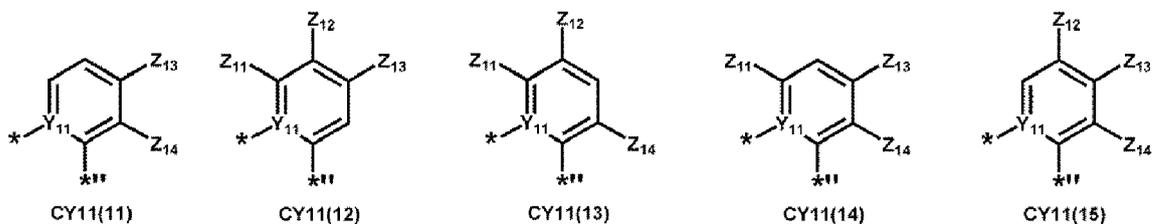
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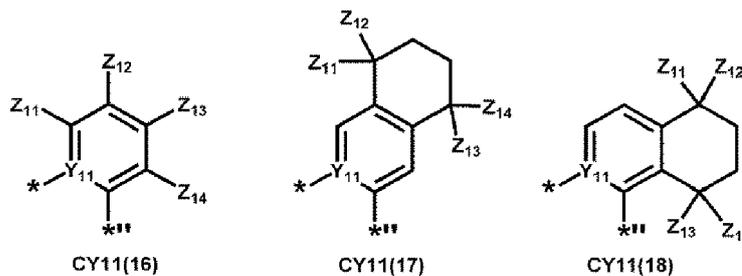


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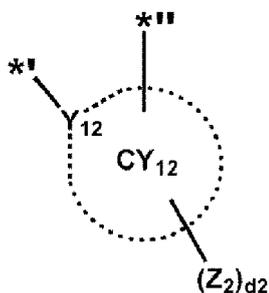
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wherein, in Formulae CY11(1) to CY₁₁(18), Y₁₂ is understood by referring to the description thereof in claim 1, Z₁₁ to Z₁₄ are each understood by referring to the description of Z₁ in claim 1, * indicates a binding site to M in Formula 1, and ** indicates a binding site to an adjacent atom in Formula 3.

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11. The organometallic compound of any of claims 1-10, wherein a group represented by

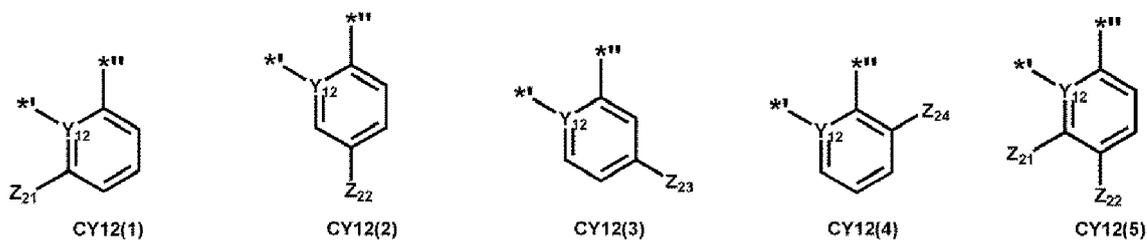
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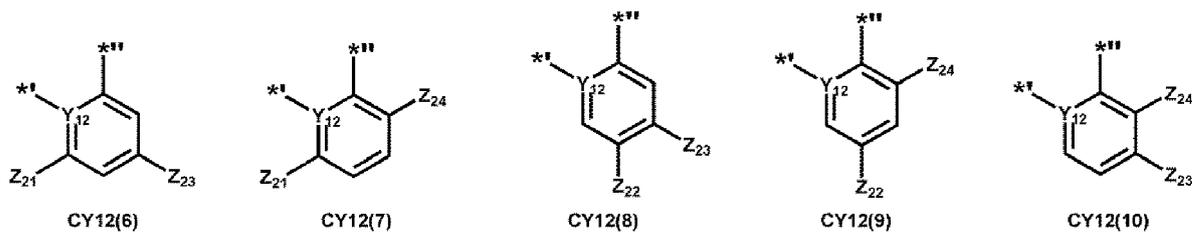
in Formula 3 is represented by one of Formulae CY12(1) to CY12(17):

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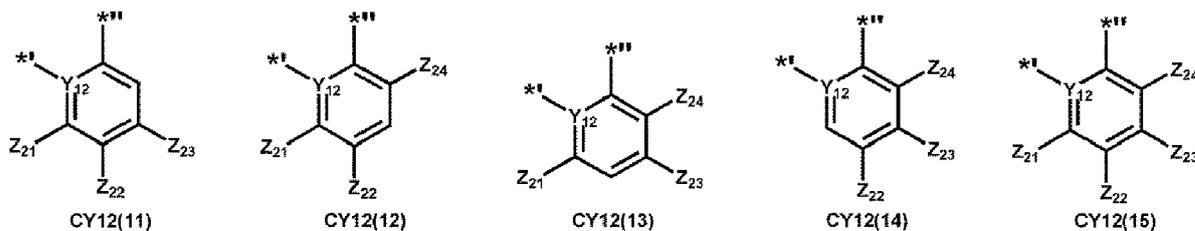
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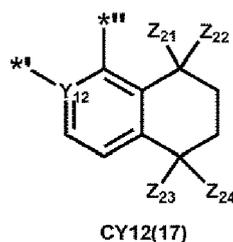
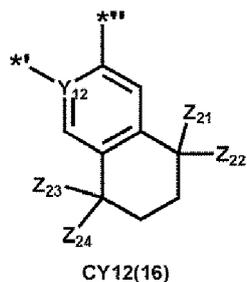
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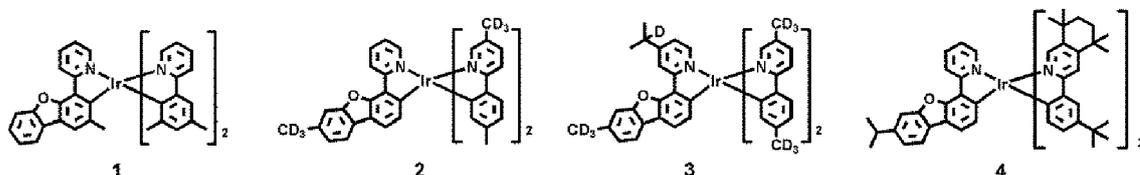
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wherein, in Formulae CY12(1) to CY12(17), Y_{12} is understood by referring to the description thereof in claim 1, Z_{21} to Z_{24} are each understood by referring to the description of Z_2 in claim 1, *' indicates a binding site to M in Formula 1, and ** indicates a binding site to an adjacent atom in Formula 3.

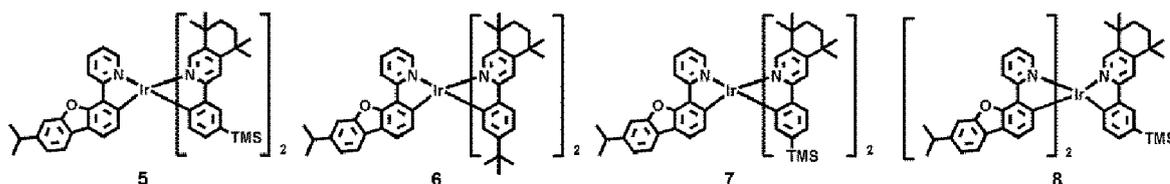
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12. The organometallic compound of claim 1, wherein the organometallic compound is of Compounds 1 to 296:

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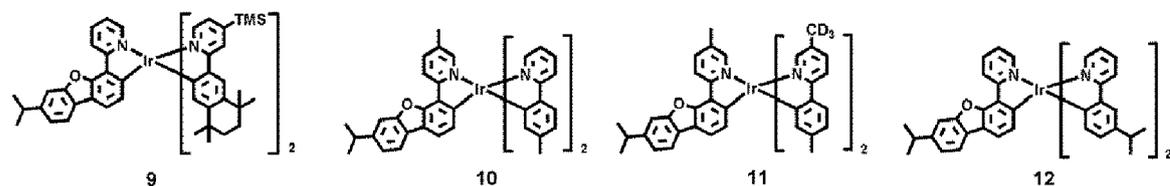


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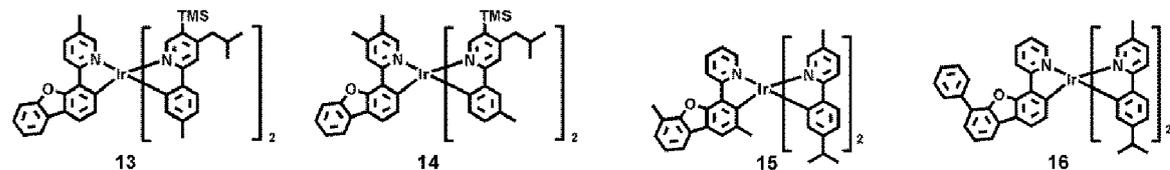


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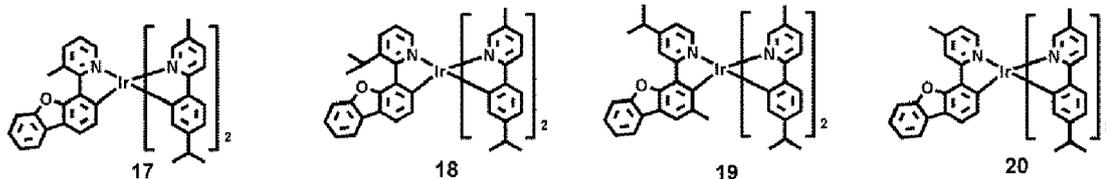


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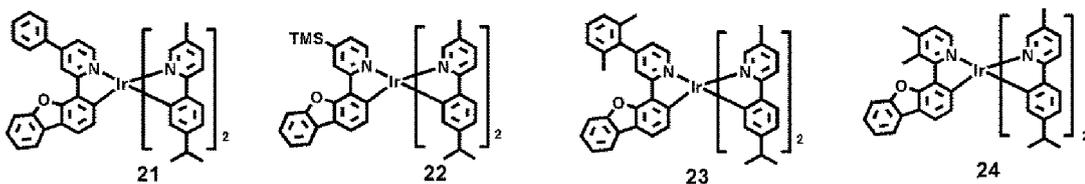


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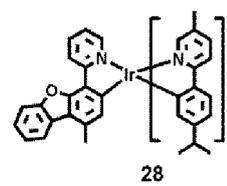
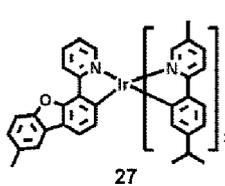
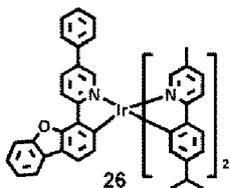
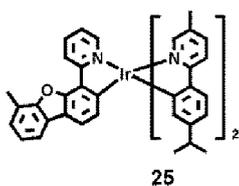
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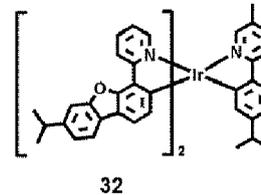
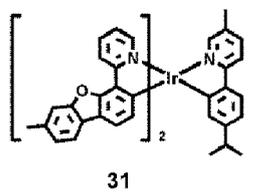
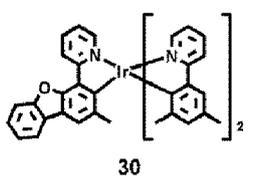
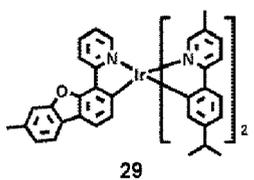
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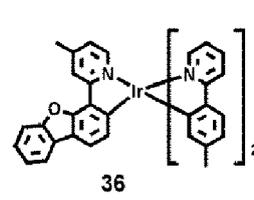
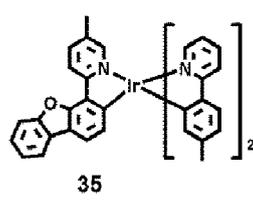
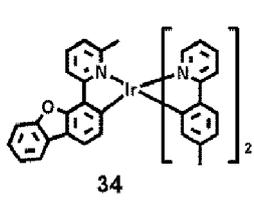
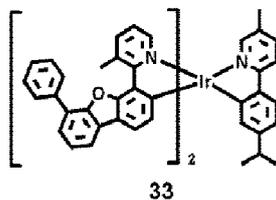
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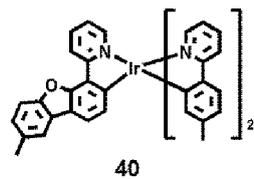
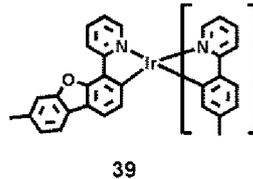
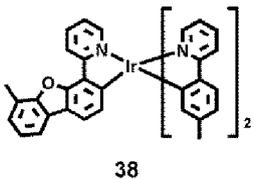
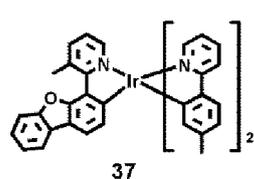
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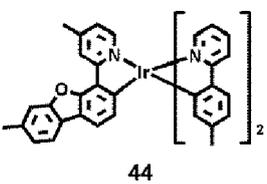
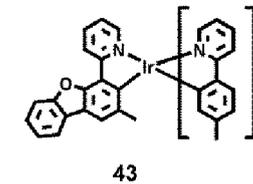
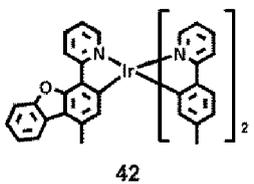
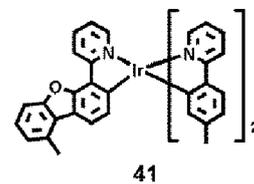


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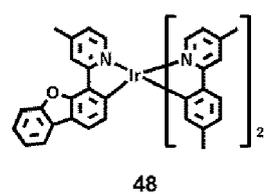
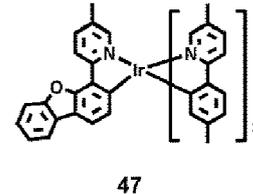
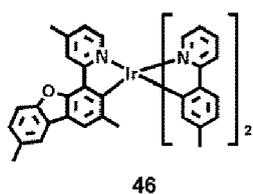
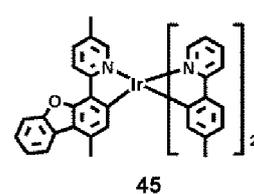
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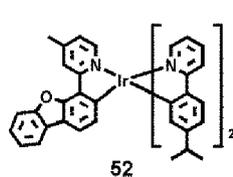
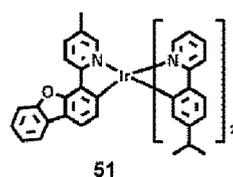
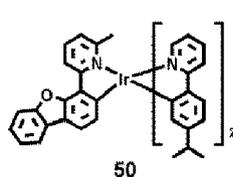
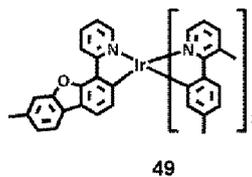
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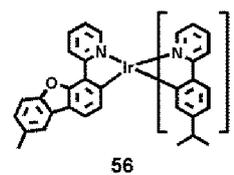
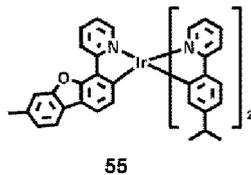
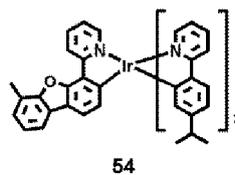
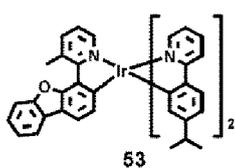
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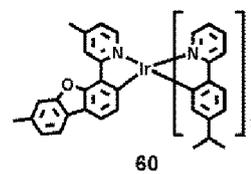
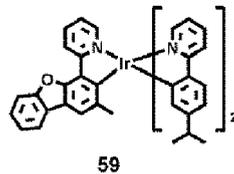
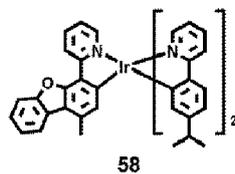
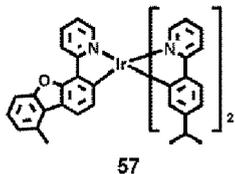


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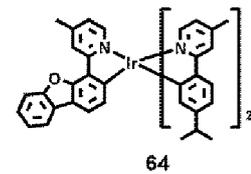
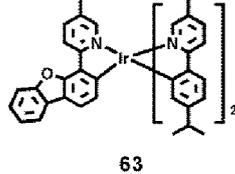
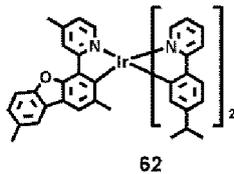
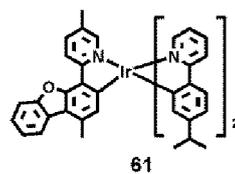
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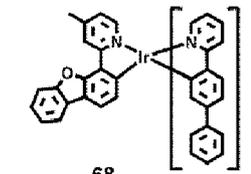
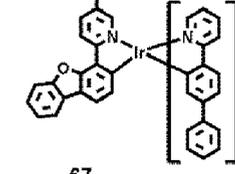
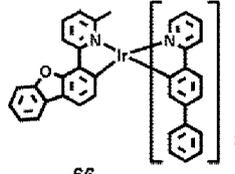
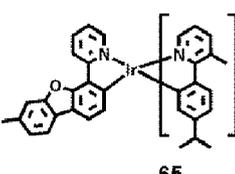
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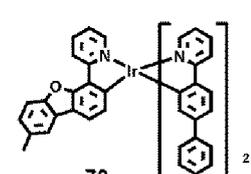
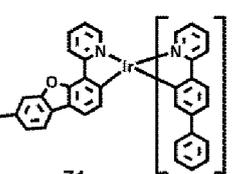
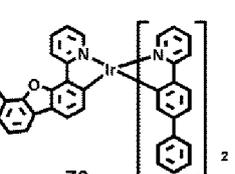
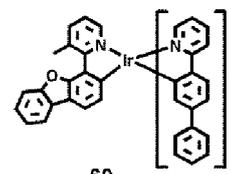
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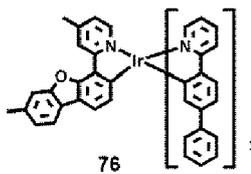
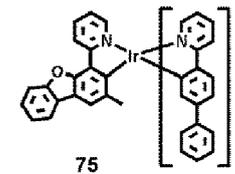
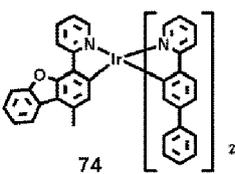
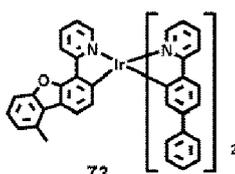
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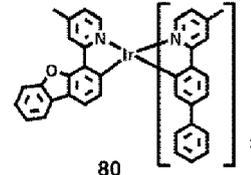
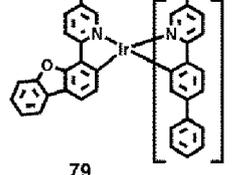
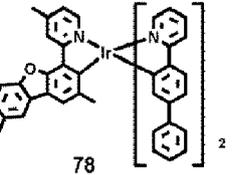
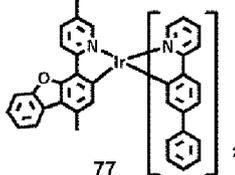
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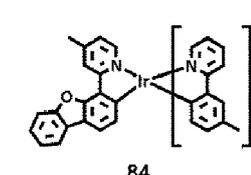
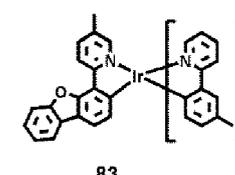
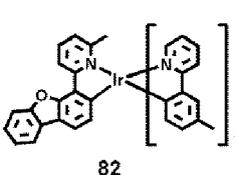
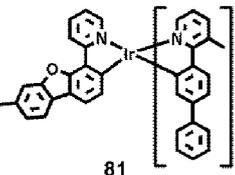
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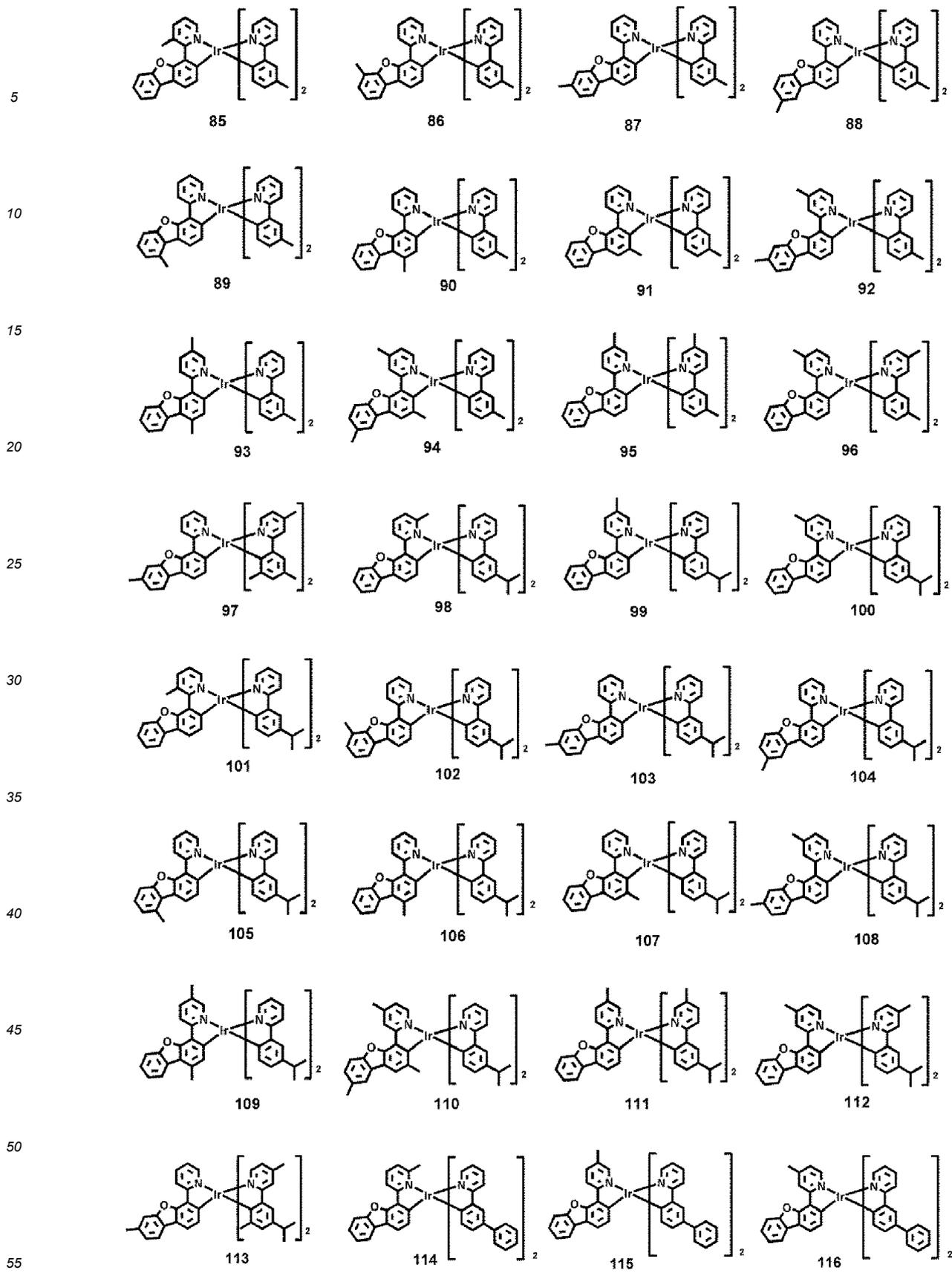
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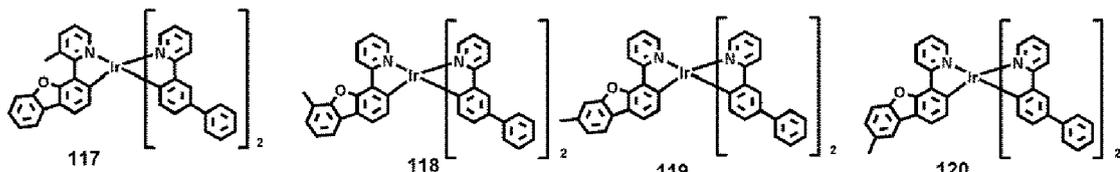
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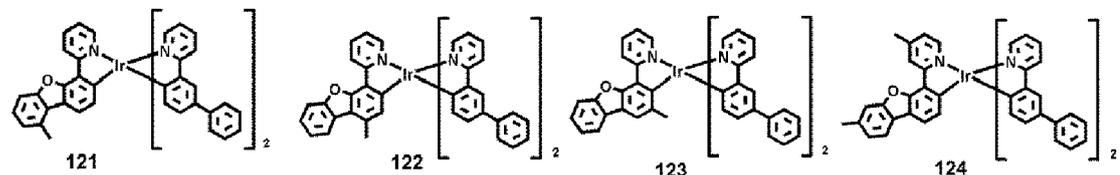
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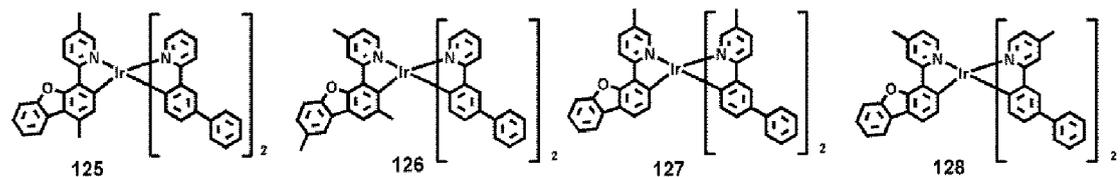
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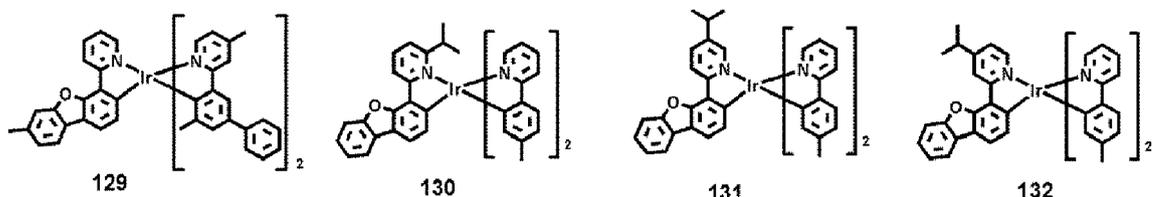
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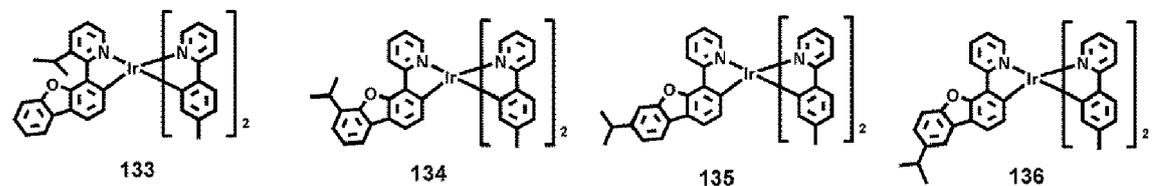


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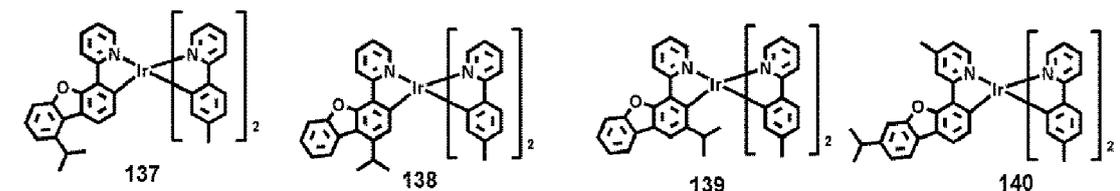
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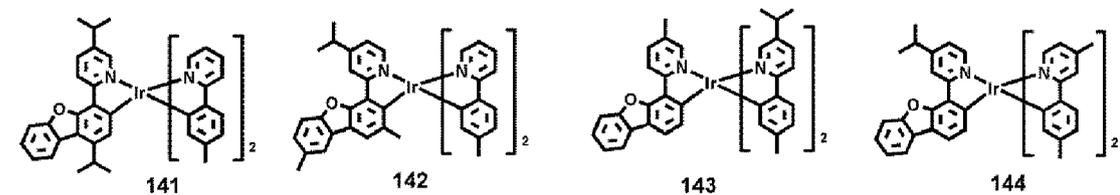
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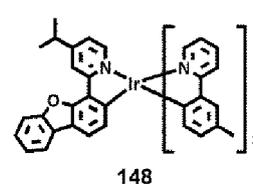
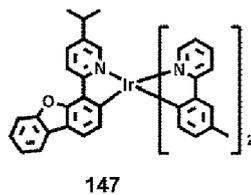
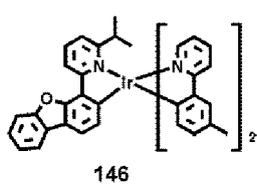
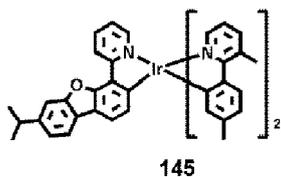
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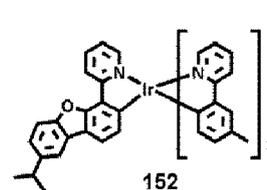
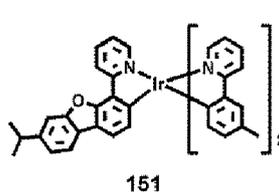
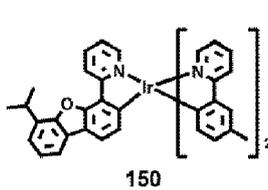
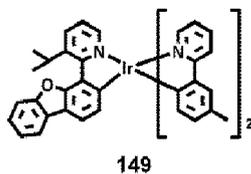


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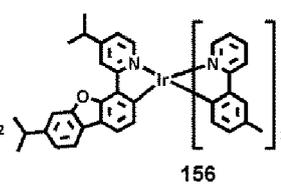
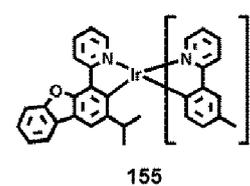
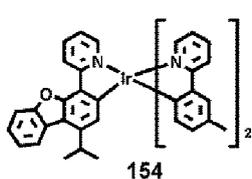
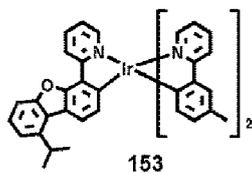
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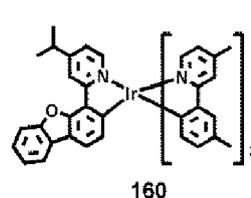
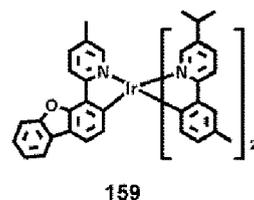
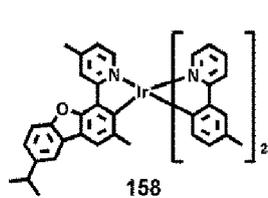
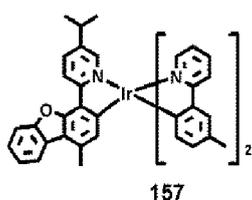
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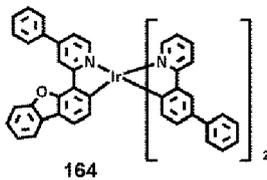
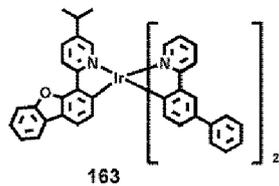
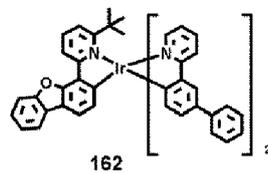
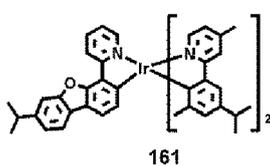


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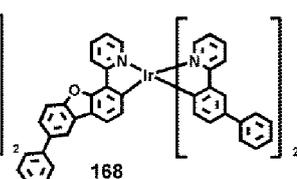
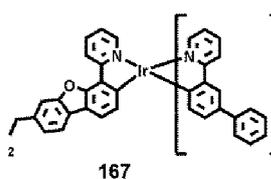
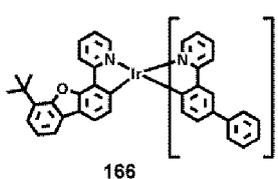
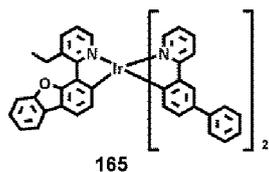
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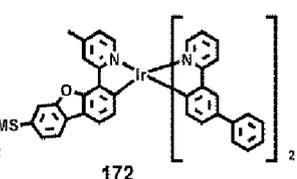
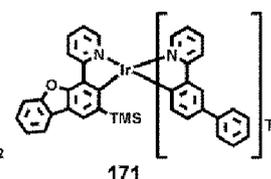
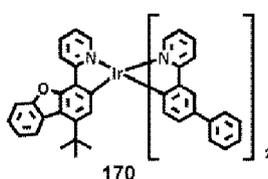
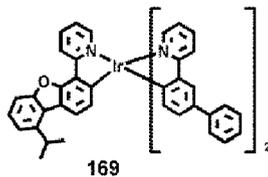
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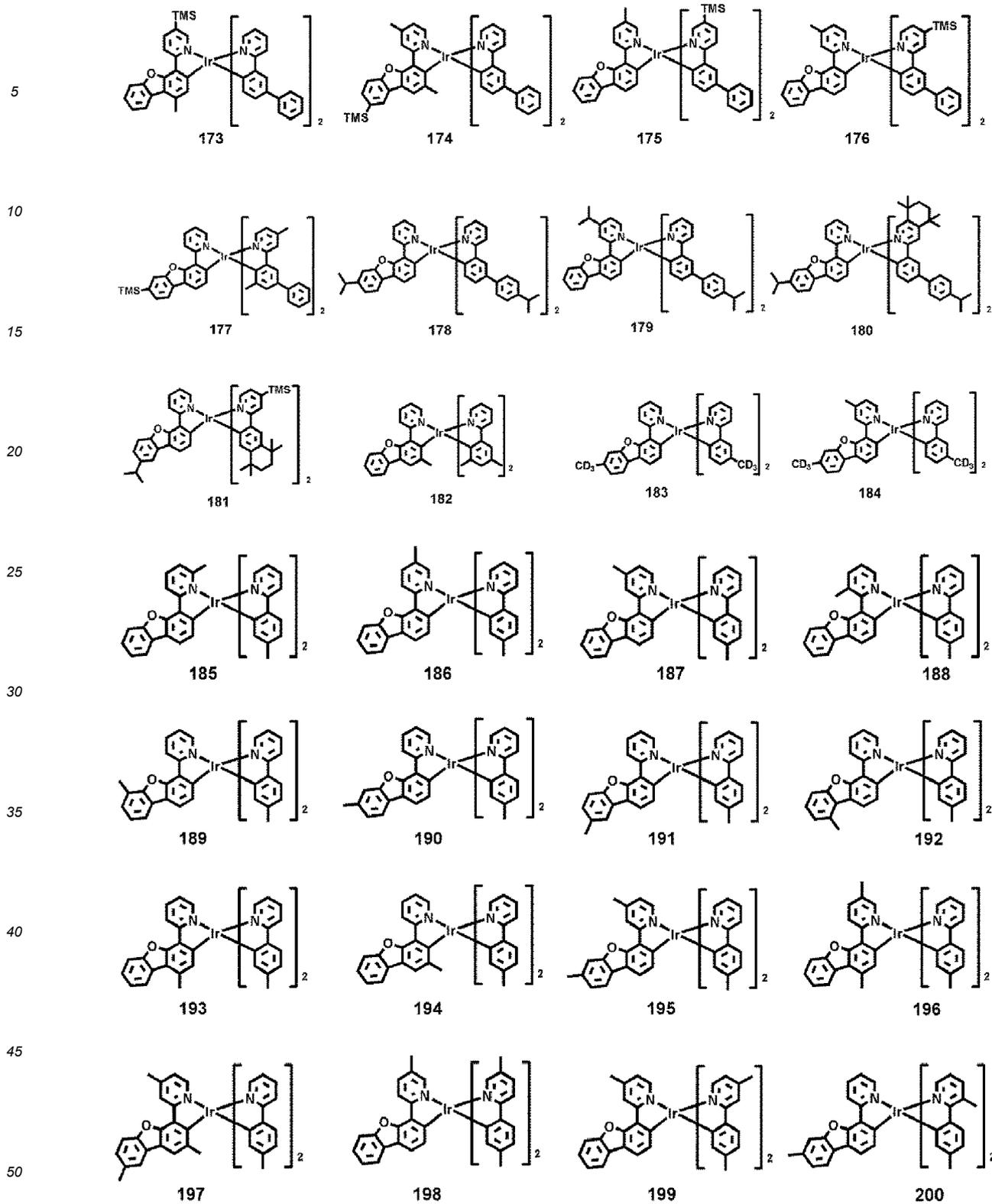


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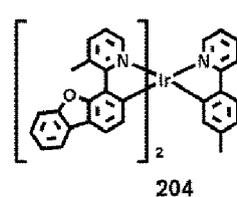
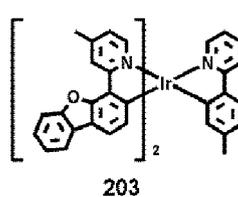
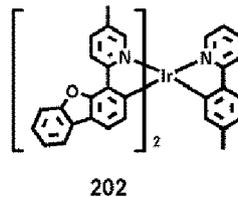
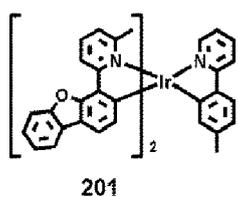
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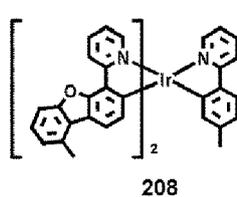
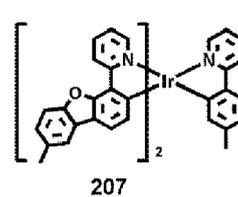
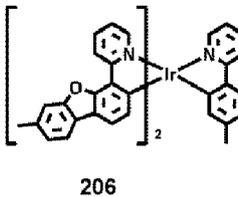
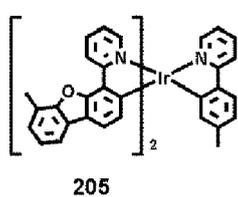
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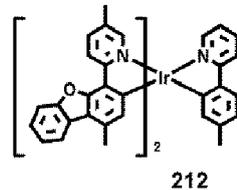
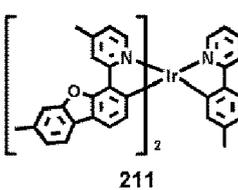
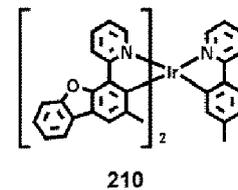
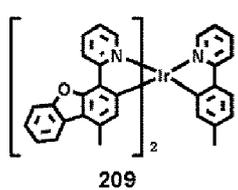
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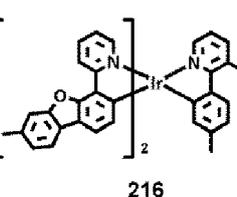
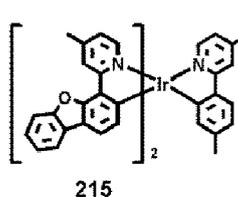
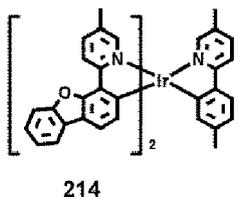
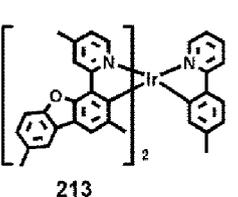
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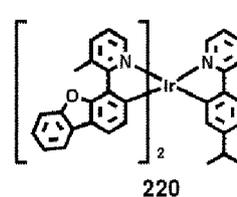
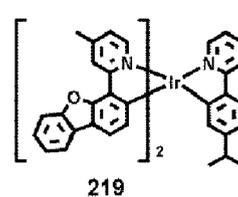
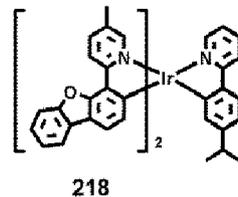
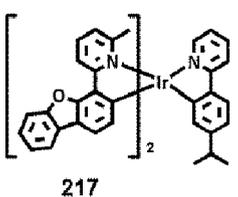


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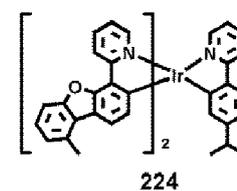
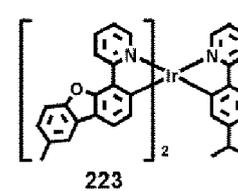
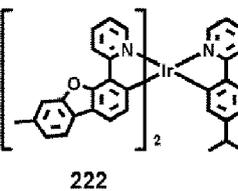
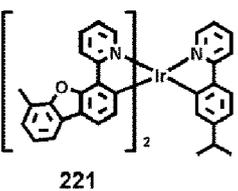
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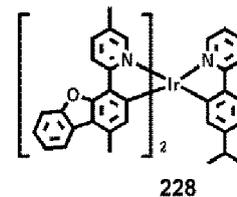
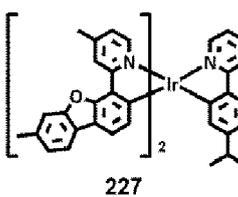
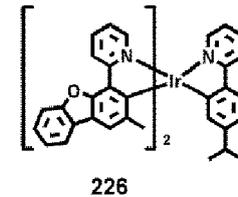
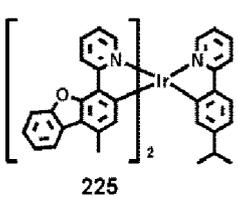
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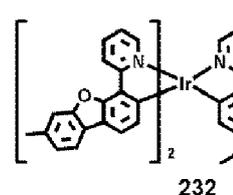
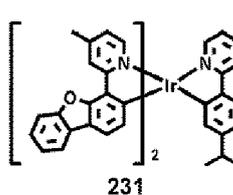
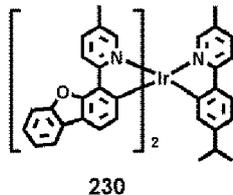
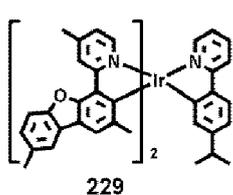
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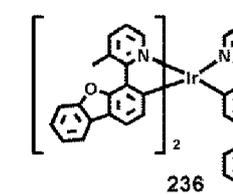
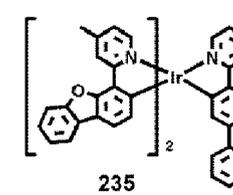
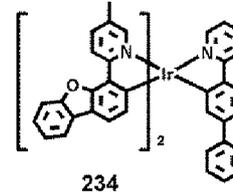
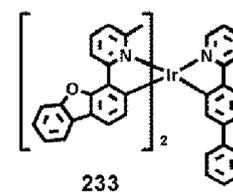


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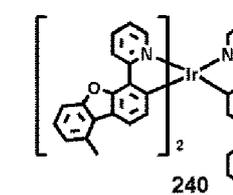
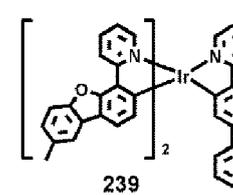
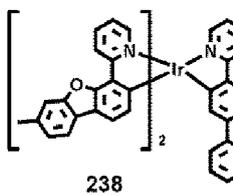
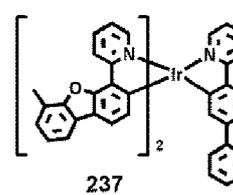


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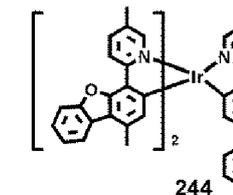
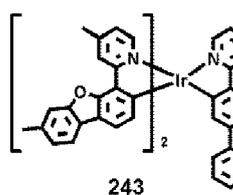
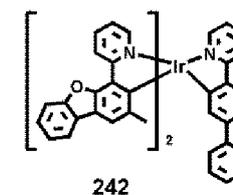
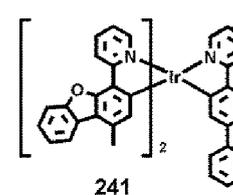
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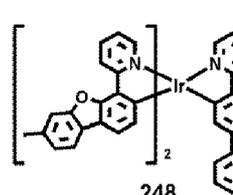
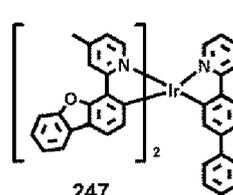
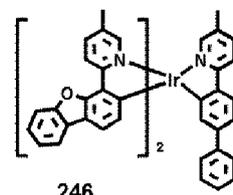
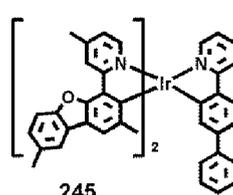
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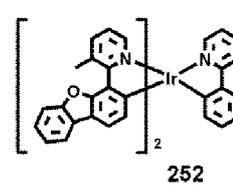
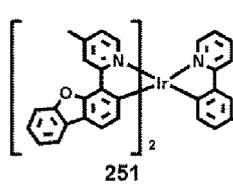
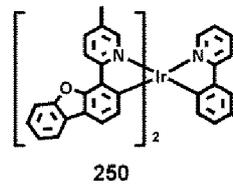
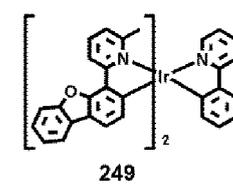


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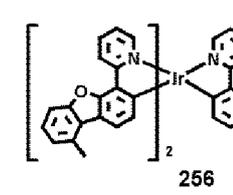
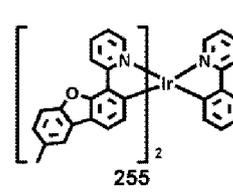
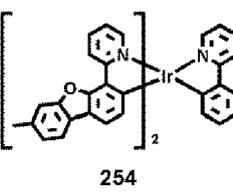
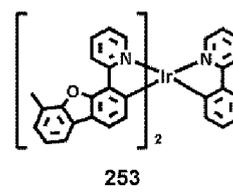
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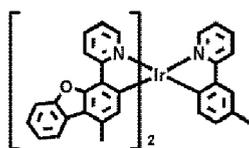


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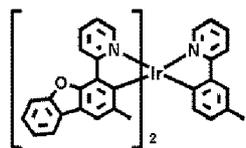


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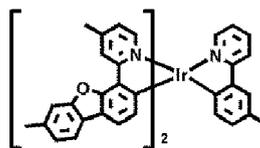
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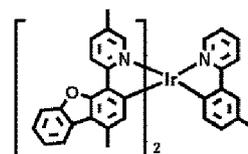
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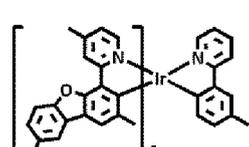


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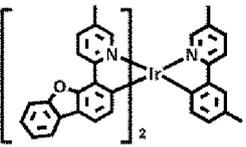


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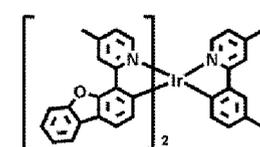
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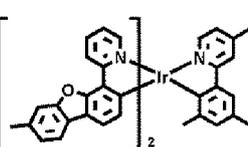
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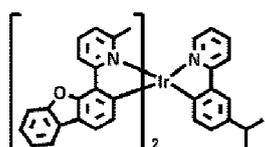


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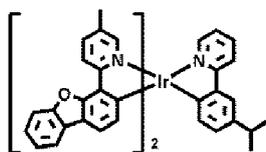


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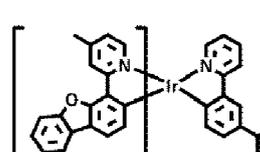
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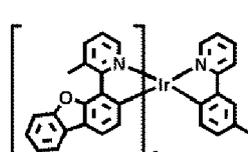
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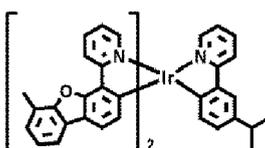


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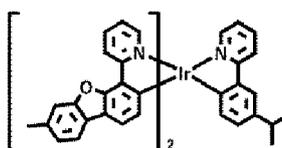


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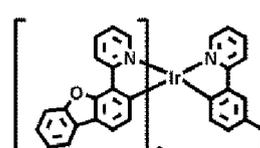
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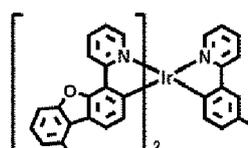
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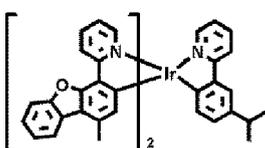


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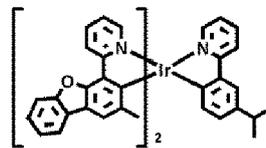


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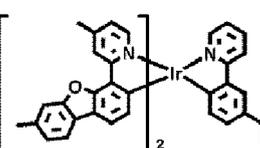
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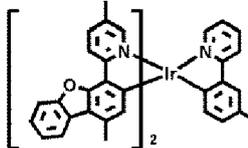
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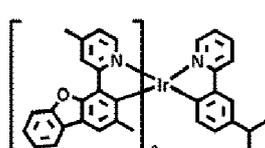


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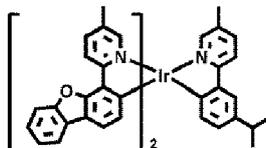


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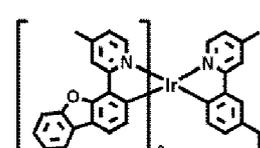
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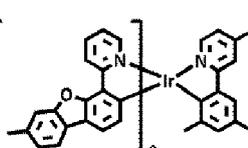
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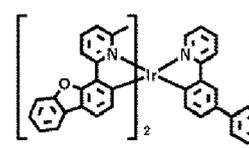


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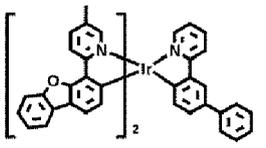


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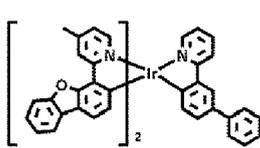
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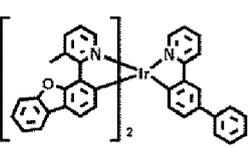
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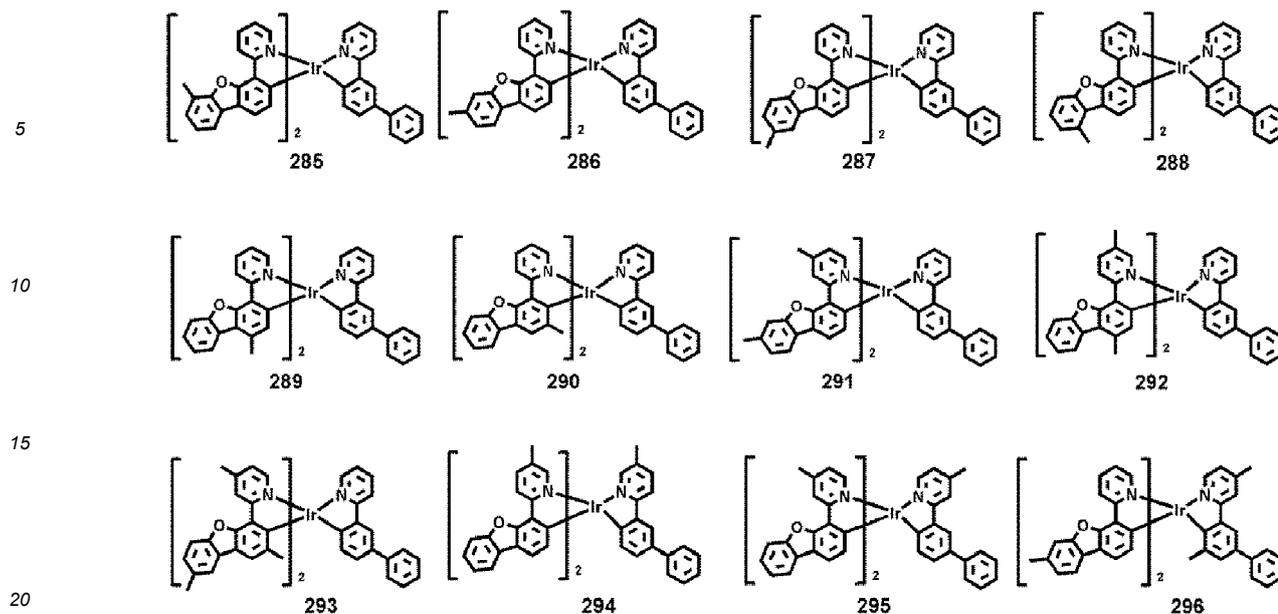
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13. An organic light-emitting device comprising:

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- a first electrode;
 - a second electrode; and
 - an organic layer disposed between the first electrode and the second electrode and comprising an emission layer; and
 - wherein, the organic layer comprises at least one organometallic compound of any of claims 1-12;
 - preferably wherein

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 - the first electrode is an anode,
 - the second electrode is a cathode, and
 - the organic layer further comprises a hole transport region disposed between the first electrode and the emission layer and an electron transport region disposed between the emission layer and the second electrode,
 - the hole transport region comprises a hole injection layer, a hole transport layer, an electron blocking layer, a buffer layer, or any combination thereof, and

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 - the electron transport region comprises a hole blocking layer, an electron transport layer, an electron injection layer, or any combination thereof.

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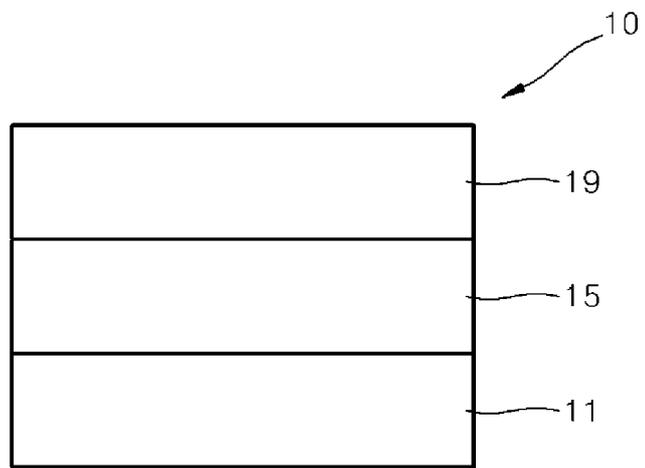
14. The organic light-emitting device of claim 13, wherein the emission layer comprises the organometallic compound; preferably wherein the emission layer further comprises a host in an amount greater than an amount of the organometallic compound.

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15. A diagnostic composition comprising one of the organometallic compounds of any of claims 1-14.

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EUROPEAN SEARCH REPORT

Application Number
EP 20 20 8566

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The present search report has been drawn up for all claims			
Place of search The Hague		Date of completion of the search 12 April 2021	Examiner Bourghida, E
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